

# Compression, inversion, and approximate PCA of dense kernel matrices at near-linear computational complexity

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**Abstract:** Dense kernel matrices  $\Theta \in \mathbb{R}^{N \times N}$  obtained from point evaluations of a covariance function  $G$  at locations  $\{x_i\}_{1 \leq i \leq N}$  arise in statistics, machine learning, and numerical analysis. For covariance functions that are Green’s functions elliptic boundary value problems and approximately equally spaced sampling points, we show how to identify a subset  $S \subset \{1, \dots, N\} \times \{1, \dots, N\}$ , with  $\#S = \mathcal{O}(N \log(N) \log^d(N/\epsilon))$ , such that the zero fill-in block-incomplete Cholesky decomposition of  $\Theta_{i,j} \mathbb{1}_{(i,j) \in S}$  is an  $\epsilon$ -approximation of  $\Theta$ . This block-factorisation can provably be obtained in  $\mathcal{O}\left(N \log^2(N) (\log(1/\epsilon) + \log^2(N))^{4d+1}\right)$  complexity in time. Numerical evidence further suggests that element-wise Cholesky decomposition with the same ordering constitutes an  $\mathcal{O}\left(N \log^2(N) \log^{2d}(N/\epsilon)\right)$  solver. The algorithm only needs to know the spatial configuration of the  $x_i$  and does not require an analytic representation of  $G$ . Furthermore, an approximate PCA with optimal rate of convergence in the operator norm can be easily read off from this decomposition. Hence, by using only subsampling and the incomplete Cholesky decomposition, we obtain at nearly linear complexity the compression, inversion and approximate PCA of a large class of covariance matrices. By inverting the order of the Cholesky decomposition we also obtain a near-linear-time solver for elliptic PDEs.

**Keywords:** Cholesky decomposition, covariance function, gamblet transform, kernel matrix, sparsity, principal component analysis.

**2010 Mathematics Subject Classification:** 65F30 (42C40, 65F50, 65N55, 65N75, 60G42, 68Q25, 68W40)

## 1 Introduction

### 1.1 A surprising phenomenon

Large dense matrices arise very frequently in applied mathematics, e.g. in machine learning, statistical inference and scientific computing more generally. Even elementary computations (such as multiplication and inversion) involving such matrices can be computationally costly, so it is naturally of interest to investigate whether approximate computations can be performed more cheaply, with a suitable tradeoff of accuracy versus computational cost. The purpose of this article is to illustrate a surprisingly simple

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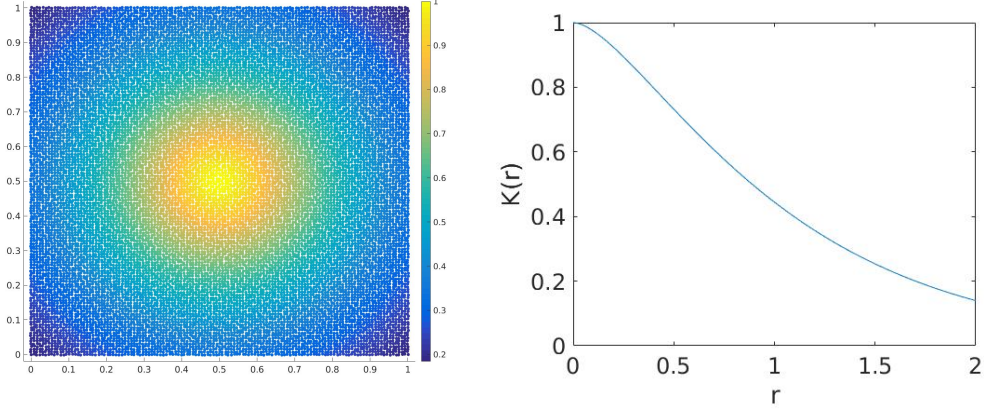


Figure 1: Point cloud and kernel. The first panel shows the cloud of evaluation points, together with the kernel function in 2D. The second panel shows the one dimensional plot of the kernel.

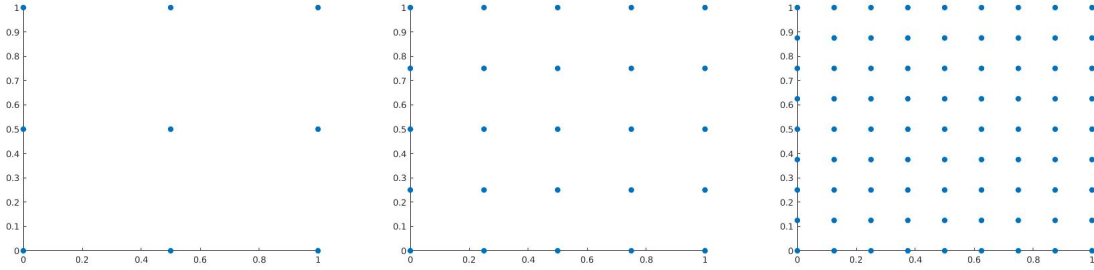


Figure 2: A nested hierarchy of point sets. These plots show an example for  $I^{(1)}, I^{(2)}, I^{(3)}$ .

and accurate sparse approximation using the incomplete Cholesky factorisation, which applies when the entries of the matrix are ‘spatially regular’ in a suitable sense.

Let us start with a prototypical example. Consider a point cloud of size  $N = 16641$ ,  $\{x_i\}_{i \in I} \subset [0, 1]^2$ , and a matrix  $\Theta_{i,j} := G(x_i, x_j) = K(\|x_i - x_j\|)$ , where  $K$  is the Matérn kernel with smoothness parameter  $\nu = 1$  and lengthscale 0.4 (Matérn, 1960; Guttorp and Gneiting, 2006), as depicted in Figure 1. Matrices of this type occur in many areas of machine learning, statistical inference and scientific computing.

Assume now, that the point set can be written as the union  $\{x_i\}_I = \bigcup_{k=1}^q \{x_i\}_{i \in I^{(k)}}$  where the  $I^{(k)}$  form a nested hierarchy of points, as depicted in Figure 2. We note, that the points on each hierarchy do not need to be exactly equidistant, we only require, for  $J^{(k)} := I^{(k)} \setminus I^{(k-1)}$ :

$$\max_{x \in [0,1]^2} \min_{j \in J^{(k)}} \text{dist}(x, x_j) \leq 2^{-k}, \quad (1.1)$$

$$\min_{i,j \in \bigcup_{1 \leq l \leq k} J^{(l)}} \text{dist}(x_i, x_j) \geq \delta_{\text{mesh}} 2^{-k}, \quad (1.2)$$

for a  $\delta_{\text{mesh}}$  not too small. Now define the set

$$S_2 := \left\{ (i, j) \in I \times I \mid i \in J^{(k)}, j \in J^{(l)}, \text{dist}(x_i, x_j) \leq 2 * 2^{\min(k,l)} \right\}.$$

Assume that the index set of  $\Theta$  is ordered such that  $l < k \Rightarrow (i \in J^{(l)}, j \in J^{(k)} \Rightarrow i \prec j)$ . We now define

$$\tilde{\Theta}_{i,j} := \begin{cases} \Theta_{i,j}, & \text{for } (i, j) \in S_2 \\ 0, & \text{else} \end{cases} \quad (1.3)$$

In our example, we have  $\#S = 5528749 = 0.0189N^2$ , which means that most of the entries of  $\tilde{\Theta}$  are zero, as illustrated in figure Now we want to investigate, how much information of the original  $\Theta$  is still

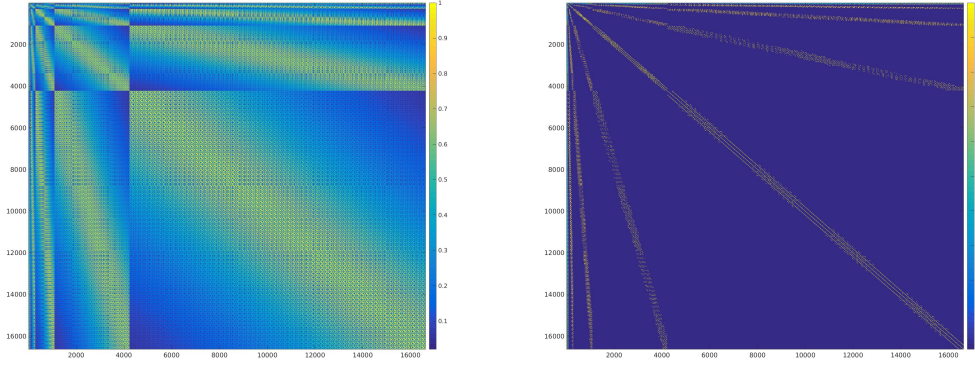


Figure 3: Comparison of  $\Theta$  and  $\tilde{\Theta}$ . The left panel shows the original, dense kernel matrix. The right panel shows its truncation to  $S_2$ .

contained in its truncation,  $\tilde{\Theta}$ . To this end, we compute the relative error in operator norm, and obtain:

$$\frac{\|\Theta - \tilde{\Theta}\|}{\|\Theta\|} = 0.9662. \quad (1.4)$$

This poor approximation ratio is not surprising, since we have thrown away all but 1.89% of the entries. The question that arises, is whether we can extract more information from these 1.89% of entries. It turns out that this is possible with a very simple algorithm. Let  $\tilde{L}$  be the incomplete Cholesky factor of  $\tilde{\Theta}$ , that is the result of a Cholesky factorisation of  $\tilde{\Theta}$ , where all read- and write operations on  $S_2$  are skipped. We obtain the following relative approximation error:

$$\frac{\|\Theta - \tilde{L}\tilde{L}^T\|}{\|\Theta\|} = 3.0676\text{e-}04, \quad (1.5)$$

thus yielding a very accurate approximation of the original covariance matrix, even though the factor  $\tilde{L}$  has the same sparsity pattern as  $\tilde{\Theta}$ .

One purpose of this paper is to show that the phenomenon illustrated by the above example is generic, i.e. we will show that the phenomenon described above. (a) holds true for a large class of covariance functions  $G$  (including Green's function of elliptic boundary value problems); (b) leads to near-linear complexity approximate sparse 'Cholesky decomposition and PCA' of the associated covariance matrices  $\Theta$ ; and (c) results in near-linear complexity direct solvers for elliptic PDEs with rough coefficients.

Our approach is based on the *gamblet* multi-resolution analysis developed by Owhadi (2017) and Owhadi and Scovel (2017), which we will, to some degree, generalize. Another purpose of this paper is to further illustrate interplays between Gaussian random fields, Gaussian elimination, statistical inference, numerical homogenisation and multi-resolution methods.

## 1.2 Computing with dense kernel matrices

Symmetric positive definite matrices of the form

$$\Theta_{i,j} := \iint_{\Omega} v_i(x) G(x,y) v_j(y) \, dx \, dy$$

play an important role in many different parts of applied mathematics. In numerical analysis, these matrices arise as discretised integral operators and are obtained by integrating the Green's function  $G$  of a partial differential operator against test functions  $\{v_i\}_i$  (Hsiao, 2006; Sauter and Schwab, 2011). In computer graphics, the radiosity equation describing the illumination of a scene is an integral equation of the above kind (Gortler et al., 1993). In machine learning, replacing the Gram matrix of the

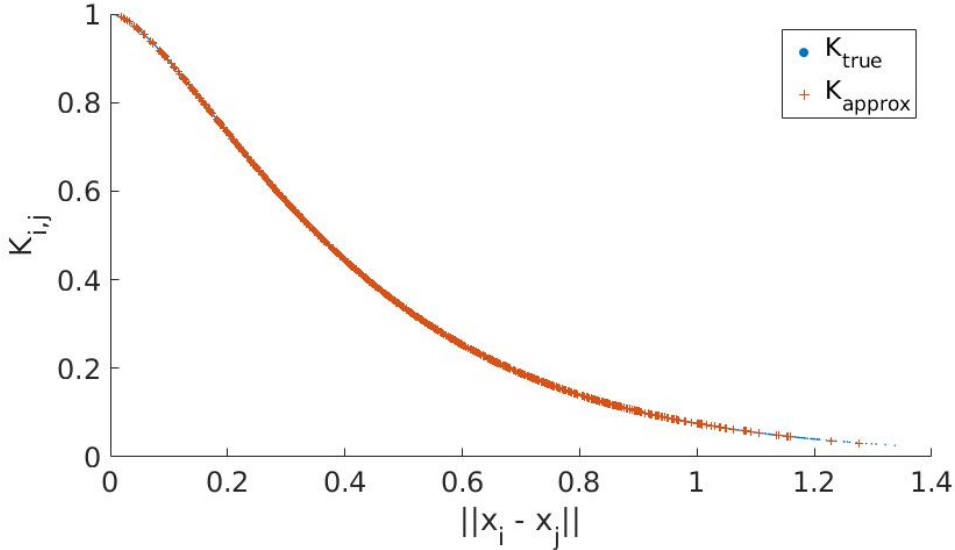


Figure 4: Comparison of  $\Theta$  and  $\tilde{\Theta}$ . Each point in this scatterplot corresponds to a pair of sampling points  $x_i, x_j$ . On the  $x$ -axis the distance between the points is plotted and on the  $y$ -axis the corresponding  $\Theta_{i,j}$  (blue) or  $\tilde{\Theta}_{i,j}$  (red) is plotted.

measurement vectors by a kernel matrix of the above form often allows one to implicitly work in an infinite dimensional feature space (Schölkopf and Smola, 2002). Kernel matrices also play a central role in *scattered data approximation* (Wendland, 2005), i.e. function interpolation based on unstructured localised measurements. Finally, since covariance matrices of Gaussian processes are kernel matrices, such matrices also play a central role in spatial-statistical methods such as Kriging (Stein, 1999).

The examples presented above typically require multiplying vectors by  $\Theta$  or its inverse or the computation of  $\det(\Theta)$ . Since integral operators are typically nonlocal, the resulting matrices will generally be dense. Recall that when  $\Theta$  is a  $N \times N$  matrix, standard Gaussian elimination methods to compute the inverse and determinant would be of  $\mathcal{O}(N^3)$  complexity and even a matrix-vector multiplication involving  $\Theta$  will have complexity  $\mathcal{O}(N^2)$ . For large  $N$ , this cubic cost is prohibitively high, making it necessary to exploit the structure of the underlying problem.

### 1.3 Existing methods

Kernel-based approaches are ubiquitous in applied mathematics and there is a rich literature on methods designed to avoid the  $\mathcal{O}(N^3)$  bottleneck incurred by vanilla solvers that are based upon Gaussian elimination. Although this brief review is not exhaustive, we will try to provide an overview of existing techniques, loosely sorted by field of application and underlying ideas.

The simplest way of approximating large kernel matrices is subsampling. The underlying idea is that subsampled data points may contain enough information to achieve the desired accuracy. Furthermore, if parts of the domain require more accurate estimates, points in these regions can be adaptively sampled at a higher rate. In the Gaussian process statistics community, this approach is frequently referred to as the selection of an *active set* of training variables (Rasmussen and Williams, 2006). From the point of view of the kernel matrix, subsampling the data just amounts to subsampling rows and columns. Some algorithms proposed for this purpose rely on greedy selection combined with a cheap estimator for the quality of the approximation (Smola and Schölkopf, 2000; Bach and Jordan, 2003; Fine and Scheinberg, 2001). When solving integral equations arising in PDEs, the user usually has more flexibility in choosing the mesh of the discretisation than the statistician has in choosing the measurement locations of the training data. From this point of view, (adaptive) mesh generation amounts to subsampling an infinite amount of data (Feischl et al., 2015).

Subsampling schemes, which correspond to subsampling the rows and columns of the covariance ma-

trix, can also be seen as low rank approximations, with the additional restriction that the low dimensional subspace must be spanned by a set of vectors of the standard basis. Although individual measurements define non-adapted bases, fixed-rank Kriging can be used to produce adapted bases (Cressie and Johannesson, 2008). In some problems, the prior knowledge of a good separable approximation of the kernel function may inform the choice of a low rank model. An initial subsampling procedure can also be combined with an eigendecomposition (Williams and Seeger, 2001; Santin and Schaback, 2016) to improve the accuracy of the low rank approximation. This approach is in some sense similar to that of Halko et al. (2011), where a random projection followed by an SVD is used to obtain low rank approximations of matrices. Another probabilistic algorithm is given by Rahimi and Recht (2008) and relies on the *inverse* kernel trick together with random projections to approximate the kernel matrix by the Gram matrix of a low dimensional feature map. Chalupka et al. (2013) compare approximation methods for Gaussian process regression and Stein (2014) shows that low rank models can perform poorly even in presence of strong correlation between neighbouring points.

A way to overcome the limitations of low rank approximations is to recognise that long-range correlations tend to be of lower rank than short-range correlation. Therefore, adapting the rank of the approximation to submatrices may be a better strategy. Using this idea in the context of particle simulations, the pioneering work of Greengard and Rokhlin (1987) shows that it is possible to apply dense kernel matrices to vectors in  $\mathcal{O}(N)$  time, with rigorous error estimates. As an abstraction of those ideas, the concept of *hierarchical matrices* was developed (Hackbusch and Khoromskij, 2000; Hackbusch, 1999; Hackbusch and Börm, 2002; Börm et al., 2003). Hierarchical matrices provide a framework for efficiently computing with matrices that have large low rank submatrices and have been successfully used as fast solvers for PDEs (Bebendorf, 2016, 2008). Despite their various favorable properties (including the existence of rigorous error estimates for a wide range of problems), the spread of these methods appear to have remained limited in the statistics community. Nevertheless, as recently described by Ambikasaran et al. (2016), these methods are well suited for many standard problems arising in Gaussian process statistics.

Although the approximation methods discussed above are all based on low rank properties, there is another class of methods, often called *covariance tapering*, that artificially imposes sparsity by truncating long-range correlations (Furrer et al., 2006). While this may seem like a very crude approximation, it is empirically known to perform well (Chilès and Delfiner, 2012; Armstrong, 1998; Journel and Huijbregts, 1978). Furrer et al. (2006) asserts that the success of covariance tapering (despite the presence of large scale correlations) could be heuristically explained by a *screening effect*. The idea of this phenomenon, analysed theoretically by Stein (2002), is that strongly correlated random variables corresponding to distant points in space may become weakly correlated after conditioning on their neighbours (through a process of shielding). The iterative conditioning of a Gaussian process can be shown to be equivalent to computing the Cholesky decomposition of its covariance matrix and, as a result, *screening* is also a well known phenomenon in the sparse Cholesky decomposition literature, where it forms the basis of nested dissection type algorithms (George, 1973). As opposed to artificially sparsifying the covariance matrix, Lindgren et al. (2011) use the correspondence between Matérn kernels and stochastic partial differential equations as observed by Whittle (1954, 1963). They construct a fine mesh, on which they discretise the elliptic PDE associated to the Matérn covariance function considered. By performing a nested dissection Cholesky decomposition of the stiffness matrix  $\mathcal{L}$ , they obtain a computationally tractable form of  $\mathcal{L}^{-1}$ , which is then used as a covariance operator. Here, the sparsity is inherited from the locality of the associated partial differential operator. Similiar approaches, that stem from the idea to directly approximate the PDE associated to the Matérn kernel have been proposed by Roininen et al. (2011, 2013, 2014) in the context of Bayesian inverse problems. In a similiar spirit, Stuart (2010) proposes the use of negative powers of “*Laplacian-like*” operators, where the size of the (possibly fractional) exponent parametrises possible a-priori beliefs regarding the smoothness of the target of estimation.

The above-mentioned idea of “conditional sparsity” leads to the next class of methods, which is often referred to as the method of *inducing variables*. As was observed in Quiñonero-Candela and Rasmussen (2005), these methods, implicitly or explicitly, cover a wide range of techniques for the sparse approximation of gaussian processes. In fact, according to Quiñonero-Candela and Rasmussen (2005), many techniques for approximate estimation with a given prior in fact amount to exact estimation with an approximate prior. This approximate prior is usually such that marginalisation with respect to a few latent variables (which can, but need not, correspond to individual measurements) results in a sparse

conditional distribution. The methods of Schwaighofer and Tresp (2003) and Snelson and Ghahramani (2006) fit into this framework. Titsias (2009) provides a variational approach for choosing induction variables. Stein et al. (2004) approximates densities via factorisations of conditional densities.

In a similar spirit, in Banerjee et al. (2008), *predictive processes*, suggested as approximations of the true process, arise from conditioning the initial process on parts of the data. Katzfuss (2016) applies this approximation hierarchically to obtain near-linear complexity approximations of the true process. Nychka et al. (2015) use hierarchies of basis functions that do not interact across scales. This idea is similar to that of using banded truncations of wavelet-transformed kernel matrices. Sang and Huang (2012) combines a low rank model for global features with a *tampered* sparse covariance for small scale interactions.

Hierarchical and multiresolution bases were introduced much earlier in numerical approximation theory (Daubechies, 1992; Mallat, 2009). We refer in particular to Beylkin et al. (1991) for the introduction of sparse wavelet based representations of integral operators. For a given approximation quality  $\varepsilon > 0$ , this allows for compression of the integral matrix in a form that enables matrix-vector multiplication with complexity  $\mathcal{O}(N \log N)$  (for the standard form of the wavelet representation) or  $\mathcal{O}(N)$  (for the non standard form).

Beylkin and Coult (1998), Beylkin (1998), and Gines et al. (1998) show how to exploit the sparsity-preserving property of the fine-to-coarse Cholesky decomposition of wavelet-based matrix representations of differential and integral operators. These methods rely on wavelets having a sufficiently high number of *vanishing moments* (i.e. their  $L^2$  orthogonality with polynomials of a given order). For a large class of boundary integral operators, Dahmen et al. (2006) prove the optimal asymptotic complexity of wavelet-based compression; see also Stevenson (2009) for a recent overview. Gantumur and Stevenson (2006) and Harbrecht and Schneider (2006) discuss the details of the implementation of such schemes.

## 1.4 Our contribution and outline of the paper

Using the estimates of Owhadi and Scovel (2017), we will show that kernel matrices obtained from local measurements of Green’s functions, and represented in a multiresolution basis, have exponentially localised Cholesky factors. Given an symmetric positive definite operator  $\mathcal{T}$  mapping a Banach space  $\mathcal{B}$  into its dual space  $\mathcal{B}^*$ , the gamblet transform developed by Owhadi and Scovel (2017) computes operator adapted wavelets (so-called gamblets) that enable a block-diagonalisation of  $\mathcal{T}$  into sparse blocks of uniformly bounded condition number. These operator-adapted wavelets define a multiresolution decomposition of  $\mathcal{B}$  obtained through the transformation of a multiresolution decomposition of  $\mathcal{B}^*$  (i.e. a hierarchy of linearly nested elements of  $\mathcal{B}^*$ ). By removing the vanishing moments conditions on the multiresolution decomposition of  $\mathcal{B}^*$  — which Owhadi and Scovel (2017) use to prove that the blocks are uniformly well conditioned — we will extend the results of Owhadi and Scovel (2017) and show that, assuming the continuity of the Green’s function, a simple subsampling scheme can be used to produce the multiresolution decomposition of  $\mathcal{B}^*$  (required by the gamblet transform and our method). Therefore, the multiresolution representation of the kernel matrix used by our method corresponds to a simple permutation of its rows and columns and results in a block-Cholesky factorisation based algorithm, that does not require the implementation of quadrature formulae, and whose overall complexity is  $\mathcal{O}(N \log^2(N) (\log(1/\epsilon) + \log^2(N))^{4d+1})$  in time and  $\mathcal{O}(N \log(N) \log^d(N/\epsilon))$  in space. As a result, given a target approximation error  $\epsilon$ , only  $\mathcal{O}(N \log(N) \log^d(N/\epsilon))$  entries need to be read (known) and those entries are solely determined by the locations of the evaluation points — in particular, they are independent of the underlying kernel. Numerical experiments suggest, that this algorithm can be replaced by simple incomplete Cholesky decomposition, decreasing the complexity in time to  $\mathcal{O}(N \log^2 N \log^{2d}(N/\epsilon))$ . Furthermore, by stopping the factorisation at step  $k$ , one obtains the  $k$  first components of a sparse approximate PCA of the covariance operator. Finally we will show that by inverting the order of elimination, one obtains a sparse factorisation of the precision matrix  $\Theta^{-1}$ . This leads to a direct solver for elliptic PDEs with rough coefficients, with complexity  $\mathcal{O}(N \log^2(N) (\log(1/\epsilon) + \log^2(N))^{4d+1})$  in time and  $\mathcal{O}(N \log(N) \log^d(N/\epsilon))$  in space. Again, based on numerical evidence, element-wise incomplete Cholesky decomposition seems to provide the same order of approximation algorithm with time complexity of only  $\mathcal{O}(N \log^2 N \log^{2d}(N/\epsilon))$ .

In Section 2 we introduce algorithms based on the exponential localisation of Cholesky factors and

describe their emergence from the interplay between statistical estimation, Gaussian elimination and numerical homogenisation. In Section 3, we rigorously prove the decay of the Cholesky factors and the overall complexity of our algorithm under general conditions. In particular, we show that matrices obtained from Green's functions of elliptic boundary value problems fulfill those general conditions if the density of the samples is homogeneous. In Section 4, we briefly discuss the practical implementation of the algorithm and provide numerical illustrations of the exponential decay. Our numerical results are based on the popular Matérn kernels which, although strictly speaking not within the scope of our theoretical results, exhibit the exponential decay predicted by our theory, with the exception of points close to the boundary. Surprisingly, this also holds true for Matérn kernels corresponding to fractional order PDEs. We summarise our results in Section 5 and discuss their relations to other available numerical methods for the treatment of kernel matrices. To conclude, we provide a brief outlook on related topics for further investigation.

The scripts and Matlab functions that were used to create the numerical experiments described in this paper can be found at

<https://github.com/f-t-s/nearLinKernel.git>

## 2 Description of the Algorithm

### 2.1 Setting

Let  $\Theta \in \mathbb{R}^{I \times I}$  be a  $I \times I$  symmetric positive definite matrix. Assume that  $\Theta$  is obtained as the Gram matrix of a positive definite kernel  $G: \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ , i.e.

$$\Theta_{i,j} := \iint \phi_i(x) G(x, y) \phi_j(y) \, dx \, dy. \quad (2.1)$$

where the  $\phi_i$  are test functionals compact and disjoint support. In this section, we will use the one dimensional Matérn kernel with smoothness  $1/2$  (i.e.  $G(x, y) := \exp(-|x - y|/\rho)$ ) as our running example to describe the sequence of ideas leading to our algorithm. We will also use Dirac delta functions as test functionals, i.e.  $\phi_i := \delta_{x_i}$  with a point cloud of  $\{x_i\}_{1 \leq i \leq N} \subset [0, 1]$  such that  $x_1 = 0$ ,  $x_N = 1$  and such that the ratio between the minimal and maximal spacing between consecutive points is bounded from above by  $\delta_{\text{mesh}}$ .

Inverting the resulting Gram matrix  $\Theta$  by the standard Cholesky decomposition has computational complexity  $\mathcal{O}(N^3)$  in time and  $\mathcal{O}(N^2)$  in space. This is frequently referred to as the  $\mathcal{O}(N^3)$ -bottleneck in Gaussian process statistics.

### 2.2 Disintegration of Gaussian measures and the screening effect

We will now show that the representation of the Gram matrix as the covariance matrix of centered Gaussian vector can be used to improve the complexity of the standard Cholesky decomposition. Recall that, since  $\Theta$  is symmetric and positive, there exists a centered Gaussian random vector  $X$  with covariance matrix  $\Theta$ , i.e.

$$\mathbb{E}[XX^T] = \Theta.$$

Recall that many integration problems in probability can be simplified by disintegration of measure. Consider for instance the problem of computing the expectation  $f(X)$  by Monte Carlo methods. For an  $X$ -measurable random variable  $Y$  we can write, using the tower property:

$$\mathbb{E}[f(X)] = \mathbb{E}[\mathbb{E}[f(X)|Y]].$$

This means that instead of sampling the random variable  $X$  directly, one can first sample  $Y$  and then sample  $(X|Y)$ . The question at this point is, of course, whether this yields any reduction in complexity. Assume for instance that  $Y$  is the Gaussian obtained by subsampling the  $X$  at entries  $i \in J$  and assume that  $J$  is limited to a single element, i.e.  $J = \{j\}$  for an element  $j$  such that  $x_j$  is close to  $\frac{1}{2}$ . Observe that  $Y$  is then just a scalar Gaussian random variable, which can be easily sampled. We will now need the following standard fact about Gaussian random vectors (see Gallier (2010), and see Owhadi and Scovel (2015) for a generalisation):



**Lemma 2.1** (Conditioning of Gaussian random variables). *Let  $X$  be a centered Gaussian random vector on  $\mathbb{R}^{n_1+n_2}$  with covariance matrix  $C$ . Assume that  $X = (X_1, X_2)$  and the corresponding block decomposition of  $C$  is*

$$C = \begin{pmatrix} C_{1,1} & C_{1,2} \\ C_{2,1} & C_{2,2} \end{pmatrix}$$

For  $x_2 \in \mathbb{R}^{n_2}$  it holds true that

$$\begin{aligned} \mathbb{E}[X_1|X_2 = x_2] &= C_{1,2}C_{2,2}^{-1}x_2, \\ \text{Cov}[X_1X_1^T|X_2 = x] &= C_{1,1} - C_{1,2}C_{2,2}^{-1}C_{2,1}. \end{aligned}$$

Let  $Z = X - Y$  and consider the problem of sampling the Gaussian vector  $(Z|Y)$ . For our example, it can be observed that the conditional covariance between  $Z_{i_1}$  and  $Z_{i_2}$  given  $Y$ , i.e.  $\text{Cov}[ZZ^T|Y]_{i_1,i_2}$ , will be close to zero if  $x_{i_1}$  and  $x_{i_2}$  are on opposite sides of  $x_j$ . This implies that  $\text{Cov}[ZZ^T|Y]$  has less than  $N^2/2$  non-negligible entries. Since the main cost in sampling a Gaussian vector consists in inverting its covariance matrix, sampling from  $(X|Y)$  might be considerably easier than sampling from  $X$ .

Observe that by conditioning on  $Y$ , we have cut the number of nonzero entries in the covariance matrix in half. What happened to the other entries of  $\mathbb{E}[\mathbb{E}[XX^T|Y]]$ ? *Fixing* the value at  $x_j$  seems to prevent values on opposite sides of it from communicating with each other. Given that the Matérn kernel is the Green's function of a PDE (Whittle, 1954, 1963; Fasshauer, 2012) this should not come as a surprise, since conditioning on  $Y$  essentially creates two independent boundary value problems. Simple linear algebra shows that this effect can always be expected if the precision matrix  $\Theta^{-1}$  is (approximately) banded. This effect is a particular instance of the *screening effect*, long known in the spatial statistics community and analysed by Stein (2002). This screening effect can be understood as a spatial Markov property that may characterise some Gaussian fields: under this property, random variables at separate locations become independent after conditioning on the variables located in between the two. The idea of exploiting *conditional* sparsity is not new and has been used to define *inducing variables* (Quiñonero-Candela and Rasmussen, 2005; Schwaighofer and Tresp, 2003) and *predictive process approximation* (Banerjee et al., 2008; Katzfuss, 2016).

### 2.3 Sparse Cholesky decomposition of dense matrices: fade-out instead of fill-in

The next idea leading to our algorithm is the equivalence of Cholesky decomposition and disintegration of Gaussian measures. The importance of this equivalence appears to have remained overlooked in the literature (apart from few instances such as Bickson (2008), where the equivalence between Cholesky decomposition and Bayesian belief propagation is explicitly used to develop a fast message passing algorithm for linear problems). In order to clarify this equivalence, we will continue working with our running example and assume that  $X^T = (Y^T, Z^T)$ . Defining  $\Theta_{11} := \mathbb{E}[YY^T]$ ,  $\Theta_{12} := \mathbb{E}[YZ^T]$ , and  $\Theta_{22} := \mathbb{E}[ZZ^T]$ , we can then write

$$\begin{aligned} \mathbb{E}[XX^T] &= \begin{pmatrix} \Theta_{11} & \Theta_{12} \\ \Theta_{21} & \Theta_{22} \end{pmatrix} = \begin{pmatrix} \text{Id} & 0 \\ \Theta_{21}\Theta_{11}^{-1} & \text{Id} \end{pmatrix} \begin{pmatrix} \Theta_{11} & 0 \\ 0 & \Theta_{22} - \Theta_{21}\Theta_{11}^{-1}\Theta_{12} \end{pmatrix} \begin{pmatrix} \text{Id} & \Theta_{11}^{-1}\Theta_{12} \\ 0 & \text{Id} \end{pmatrix} \\ &= \begin{pmatrix} \text{Id} & 0 \\ \mathbb{E}[Z|Y = \text{Id}] & \text{Id} \end{pmatrix} \begin{pmatrix} \text{Cov}[Y] & 0 \\ 0 & \text{Cov}[Z|Y] \end{pmatrix} \begin{pmatrix} \text{Id} & \mathbb{E}[Z|Y = \text{Id}]^T \\ 0 & \text{Id} \end{pmatrix}. \end{aligned}$$

For the last equality, we used Lemma 2.1 and the abuse of notation  $\mathbb{E}[Z|Y = \text{Id}]_{i,j} := \mathbb{E}[Z_i|Y = e_j]$ . Note that the above decomposition is the result of the first step of a (block-)Cholesky decomposition of  $\Theta$ .

What happens if we pick a *bisective* ordering  $i_1, i_2, \dots$  of the elements of  $I$  such that  $x_{i_1} \approx 1/2$ ,  $x_{i_2} \approx 1/4$ ,  $x_{i_3} \approx 3/4$  and so on? Figure 5 shows that as we proceed with the Cholesky decomposition of  $\Theta$ , the matrix becomes sparser. Instead of *fill-in* (i.e. the introduction of new nonzero entries), we observe a *fade-out* (i.e. the vanishing of previously nonzero entries).

Of course, our one-dimensional example has a very simple topology. How should we proceed when our test functions are living on a two-dimensional grid? The answer is to use a *quadsection* ordering as presented in Figure 6. We note that the orderings we proposed for the decomposition of  $\Theta$  are exactly



the reverse of the well known nested dissection orderings for the sparse Cholesky decomposition of sparse matrices (George, 1973; Lipton et al., 1979; Gilbert and Tarjan, 1987).

Indeed, this should not be surprise. Define  $A := \Theta^{-1}$  and assume that  $LL^T = \Theta$  is the Cholesky decomposition of  $\Theta$ . Then

$$A = (LL^T)^{-1} = L^{-T}L^{-1} \implies PAP = PL^{-T}PPL^{-1}P = (PL^{-T}P)(PL^{-T}P)^T,$$

where  $P$  is the permutation matrix reversing the order of indices. Note that multiplying from left and right by  $P$  turns upper triangular matrices into lower triangular matrices and vice versa, while keeping the number of nonzero/nonsmall entries fixed. Therefore, the Cholesky decomposition of  $A$  with reverse elimination ordering is given by  $(PL^{-T}P)(PL^{-T}P)^T$ . Furthermore, we can write  $L^{-1} = L^{-1}LL^TA = L^TA$ . If  $A$  is sparse and has at most  $l$  entries per column, then multiplication of  $L^T$  with  $A$  will increase the number of nonzero entries by at most a factor of  $l$ . Therefore, the sparsity of the Cholesky factors of  $\Theta$  with one ordering implies the sparsity of the Cholesky factors of  $A$  with the reverse order. We note that the converse is not true, as one can see by considering our one-dimensional example with the canonical ordering.

It is important to observe that the step  $\min(i, j)$  is the first time when the entry  $\Theta_{i,j}$  is used in the Cholesky decomposition. Therefore, if we know that  $\text{Cov}[X_iX_j|\{X_r\}_{1 \leq r \leq \min(i,j)}] \approx 0$ , we neither have to update nor even know the value  $\Theta_{i,j}$  to begin with. However, the set on which this is the case is only determined by the sparsity pattern of the precision matrix, not its actual value. Since this pattern is oftentimes known a priori based upon its underlying geometric structure, it can be obtained before running the actual decomposition. This allows for the sparse factorisation of  $\Theta$  in subquadratic space and subcubic time complexity if we have a good nested dissection ordering for the sparsity graph of  $(\Theta)^{-1}$ .

---

**Algorithm 1:** Sparse factorisation via reverse nested dissection ordering.

---

**Data:** A covariance matrix  $\Theta \in \mathbb{R}^{I \times I}$ , and a graph  $(I, E)$  such that  $\Theta_{i,j}^{-1} = 0$ ,  $\forall \{i, j\} \neq E$ , as well as a thickness parameter  $t$ .

**Result:** A permutation matrix  $P$  and a sparse lower triangular matrix  $L$ , such that  $PLL^TP^T = \Theta$ .

Obtain reverse nested dissection ordering  $P$  with separator thickness  $t$ . Denote its separator set by  $T$ .

Define the sparsity set

$$S := \{(i, j) | i \text{ and } j \text{ are connected in } (V, E) \text{ after removal of } \{k \in T | k < \min(i, j)\}\}.$$

Initialise the sparse matrix  $M$  as all zero.

```

for  $(i, j) \in S$  do
  if  $\Theta_{i,j} \neq 0$  then
     $M_{i,j} \leftarrow \Theta_{i,j}$ 
  else
     $M_{i,j} \leftarrow \text{eps}$ 

```

$L \leftarrow$  no fill-in incomplete Cholesky factorisation of  $M$ , with permutation  $P$

---

Here, the “thickness”  $t$  of the dissection acts as a tuning parameter that we adjust depending on the expected bandwidth of the precision matrix. The algorithm, by the same argument given by George (1973) for the factorisation of sparse matrices, has  $\mathcal{O}(N^{3/2})$  complexity in time and memory and  $\mathcal{O}(N \log N)$  complexity when using a two-dimensional regular mesh with  $t$  fixed. Thus, this simple and apparently novel algorithm already beats the  $\mathcal{O}(N^3)$  bottleneck in spatial statistics, for sparse precision matrices. We refer to Lipton et al. (1979) and Gilbert and Tarjan (1987) for extensions of the nested dissection idea to more general graphs. Lipton et al. (1979) showed that the efficiency of nested dissection depends crucially on the existence of good *separators*, in the sense that many sparse graphs without good separators are not amenable to nested dissection. While there is a rich literature on methods aimed at preventing *fill in* when applying Cholesky decomposition to sparse matrices, we are not aware of any prior work where Cholesky decomposition was used as a mean to induce sparsity. The process of conditioning, which is implicit in our algorithm, can be seen as a particular choice of *inducing points*

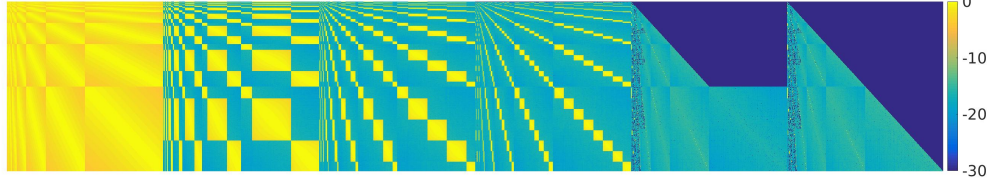


Figure 5: *Sparsification by Bisection*. As the Cholesky decomposition progresses, the entries of the remaining values (shown on a  $\log_{10}$ -scale) diminish.

according to Quiñonero-Candela and Rasmussen (2005) or *knot locations* according to Katzfuss (2016) (where, however, the connections to sparse orderings for the Cholesky decomposition do not appear to have been observed). A closely related paper is Katzfuss (2016) which proposes a multi-resolution sparse approximation of Gaussian processes, but does not use such approximations to obtain sparse matrix factorisations. Katzfuss (2016) describes good performance results in the one-dimensional setting, attributes them to the *screening effect* and suggests to choose the *knots* close to the boundaries of a partition of the space (in a way that is similar to nested dissection). Katzfuss (2016) does not, however, seem to mention that nested dissection orderings and sparse precision matrices would imply an exact sparse representation of the Gaussian process, also in higher dimensions. In closely related work, Lindgren et al. (2011) first approximate the precision matrix by a discretisation of the differential operator corresponding to the Matérn covariance function. Then they use Cholesky decomposition with a nested dissection ordering to obtain a sparse representation of the covariance operator. Based on the above arguments, for sufficiently regular sampling locations, one can instead obtain a sparse approximation by applying Cholesky factorisation with the reverse of their ordering to the covariance matrix. This avoids the explicit approximation of the precision matrix, although it might prove less stable when dealing with an inhomogeneous density of sampling points.

So far we have proposed an algorithm for the Cholesky decomposition of kernel matrices with sparse inverses and a few problems remain to be addressed:

1. Good nested dissection orderings do not always exist. In fact, the complexity of the algorithm given above is  $\mathcal{O}(N^{3/2})$  for two-dimensional meshes and deteriorates rapidly for higher-dimensional meshes.
2. The covariance matrix is usually not the inverse of a discretised partial differential operator (i.e. a sparse matrix) but is oftentimes obtained by sampling and taking local averages of the Green's function of a partial differential equation. Can the precision matrix still be approximated by a sparse matrix?

The solutions to these problems can be found in the recent literature on numerical partial differential equations, as we will see in the next section.

## 2.4 Compression, inversion and approximate PCA using gamblets

In order to resolve the above-mentioned difficulties, we will use the theory of *gamblets*, recently introduced by Owhadi (2017) and generalised by Owhadi and Scovel (2017). Although their setting is similar to ours, it is originally motivated by the problem of solving

$$\mathcal{L}u = f,$$

where  $\mathcal{L}$  is the *inverse* of  $G$  in the sense that  $\mathcal{L} \int G(x, y) f(y) = f(x)$  (i.e., from the statistical point of view,  $\mathcal{L}$  is the precision operator associated to the covariance function  $G$ ). For the sake of clarity, we will temporarily adopt the more restricted setting of Owhadi (2017), where  $\mathcal{L}$  is a second-order elliptic partial differential operator in divergence form, that is  $\mathcal{L}u(x) = -\operatorname{div}(a(x)\nabla u(x))$ . We note that many covariance functions with finite smoothness are the Green's functions of such partial differential operators. For instance, the popular Matérn kernel with smoothness  $\nu$  in dimension  $d$  is the Green's function of an

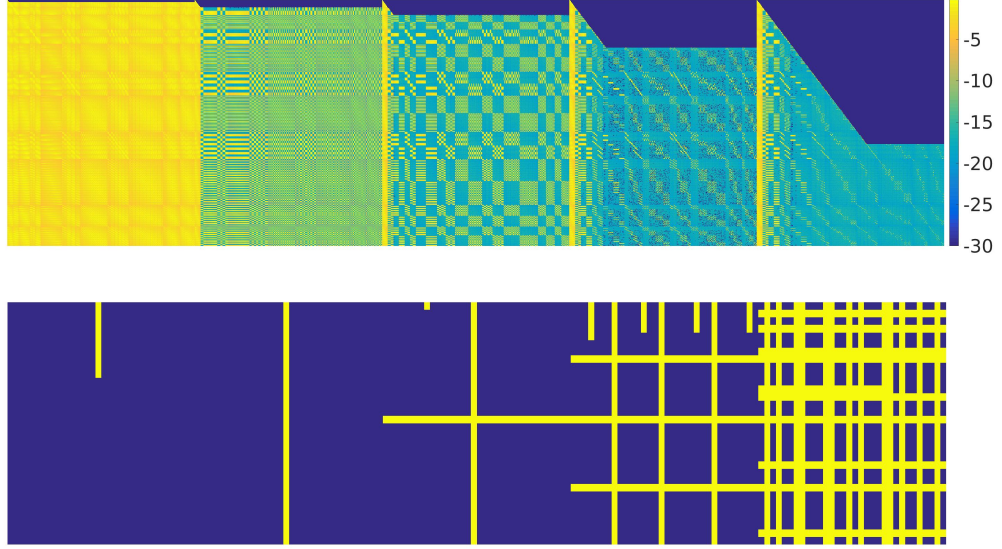


Figure 6: *Sparsification by Quadsection*. The top row shows the magnitude of the entries of  $\Theta$  (in  $\log_{10}$  scale) as the quadsective Cholesky decomposition progresses. The bottom row shows (in yellow) the positions of the indices that have been eliminated.

elliptic partial differential equation of order  $2\nu + d$  on  $\mathbb{R}^d$ , when  $\nu + d$  is an integer (Whittle, 1954, 1963; Lindgren et al., 2011; Hou and Zhang, 2017; Fasshauer, 2012).

The Galerkin (e.g. finite element) discretisation of the above equation leads to large sparse systems of linear equations. Iterative solvers such as conjugate gradient descent or the Gauss–Seidel smoother can exploit the sparsity of the discrete system. However, their convergence rate depends on the condition number of the matrix, which for partial differential equations grows as a negative power of the mesh size. Multi-grid methods (Fedorenko, 1961; Brandt, 1977; Hackbusch, 1978, 2013) are a popular way of circumventing this problem via multiscale approximations iteratively communicating via interpolation/restriction operators (the main difficulty is the identification of good interpolation operators).

Owhadi (2017) formulates the identification of good interpolation operators and the problem of computing with incomplete information as zero-sum adversarial games played against the missing information. Optimal strategies for such games are mixed (randomised) strategies, which form a saddle point for the underlying minimax problem (Owhadi and Scovel, 2017), and are identified by placing an optimal prior distribution on the solution space of the differential operator. Using this prior, the problem of estimating fine scale features of the solution based on computation on a coarser grid can then be cast as a Bayesian estimation problem.

Statistical approaches to numerical analysis are not new (Poincaré, 1987; Diaconis, 1988; Sul’din, 1959; Larkin, 1972; Sard, 1963; Kimeldorf and Wahba, 1970; Shaw, 1988; O’Hagan, 1991, 1992). However, they have in the past received little attention, and the possibilities offered by combining numerical uncertainties/errors with model uncertainties/errors (Chkrebtii et al., 2016; Owhadi, 2015; Hennig et al., 2015; Perdikaris et al., 2016; Raissi et al., 2017b; Cockayne et al., 2017) are stimulating the reemergence of such methods (Skilling, 1992; Chkrebtii et al., 2016; Schober et al., 2014; Owhadi, 2015; Hennig, 2015; Hennig et al., 2015; Briol et al., 2015; Conrad et al., 2016; Raissi et al., 2017a,b; Owhadi, 2017; Cockayne et al., 2016; Perdikaris et al., 2016; Owhadi and Scovel, 2017; Cockayne et al., 2017) where solutions of PDEs and ODEs are randomised and numerical errors are interpreted in a Bayesian framework as posterior distributions. This reemerging field is sometimes referred to as *probabilistic numerics* (Hennig et al., 2015) or *Bayesian numerical analysis* (Diaconis, 1988; Owhadi, 2015) from the Bayesian perspective or *Computational Information Games* from the game/decision theoretic perspective (Owhadi, 2017; Owhadi and Scovel, 2017).

From a Bayesian perspective, the process of randomization in probabilistic numerical methods Cock-

ayne et al. (2017) corresponds to placing a prior a distribution on the solution space of  $\mathcal{L}$  (i.e. a prior probability distribution on the *true* solution  $u$ ) and conditioning on a family of linear measurements  $[\phi_i^{(k)}, u]$  encoding the process of computing with partial information at a given resolution. From the decision theoretic perspective this prior distribution is obtained as an optimal mixed strategy for the adversarial recovery of  $u$  given the measurements  $[\phi_i^{(k)}, u]$  (Owhadi, 2017; Owhadi and Scovel, 2017). Here,  $[\cdot, \cdot]$  denotes the duality product between an element of a Banach space (second variable) and an element of its dual (first variable). Following Owhadi (2015, 2017) in the case of multiresolution methods for elliptic PDE, these functionals can be chosen as indicators functions on the elements  $\tau_i^{(k)}$  of a nested partition of the physical domain such that (1) for some  $\delta > 0$  and  $h \in (0, 1)$ , each  $\tau_i^{(k)}$  is contained in a ball of diameter  $h^k$  and contains a ball of diameter  $\delta h^k$  (2) each  $\tau_i^{(k)}$  is the union of a subset of elements  $\tau_j^{k+1}$ .

Note that the nesting of the subsets  $\tau_i^{(k)}$  implies that of the functionals  $\phi_i^{(k)}$ , i.e. there exists matrices  $\pi^{(k,l)}$  such that  $\phi_i^{(k)} = \sum_j \pi_{i,j}^{(k,l)} \phi_j^{(l)}$ , for  $k < l$ . When the relative error in operator norm  $[\mathcal{L}u, u]^{\frac{1}{2}}$  is used a loss function for the adversarial recovery problem mentioned above, the optimal mixed strategy is solely determined by the operator norm (in particular it is independent from the functionals  $\phi_i^{(k)}$ ). This optimal mixed strategy (optimal prior) is the the Gaussian field with covariance function  $G$  Owhadi and Scovel (2017) (defined as a linear isometry mapping the dual of the solution space, endowed with the dual norm of the operator norm, onto a Gaussian space).

The corresponding *best guess* for the solution  $u$ , given the measurements  $\phi_i^{(k)}$  is therefore the conditional expectation  $\mathbb{E}[u | [\phi_i^{(k)}, u]]$ . Defining the so-called *gamblets*  $\psi_i^{(k)} := \mathbb{E}[u | [\phi_j^{(k)}, u] = \delta_{i,j}]$  as the elementary conditional expectations assigned to  $\phi_i^{(k)}$ , one can write  $\mathbb{E}[u | [\phi_i^{(k)}, u]] = \sum_j [\phi_j^{(k)}, u] \psi_j^{(k)}$ .

Now, we want to split the solution space in a direct sum of gamblets on different levels. To this end, for  $k \geq 2$ , introduce the matrices  $W^{(k)}$  such that  $\text{Im}(W^{(k),T}) = \text{Ker}(\pi^{(k-1,k)})$  and  $\sum_j W_{i,j}^{(k)} \int \phi_i^{k-1} \phi_j^k = 0$ ,  $\forall i, l$ . As shown in Owhadi (2017), the  $W^{(k)}$  can be chosen such that the diameter of the support of  $\phi_i^{(k),\chi} := \sum_j W_{i,j}^{(k)} \phi_j^k$  is of order  $h^{(k)}$ . Then we define  $\chi^{(k)} := \sum_j W_{i,j}^{(k)} \psi_j^{(k)}$ . The results in (Owhadi, 2017, Theorem 3.11) show that the  $\psi_i^k, \chi_i^k$  decay exponentially, at the  $h^k$  scale, away from  $\tau_i^{(k)}$  and that the stiffness matrices  $A_{i,j}^{(k)} := [\mathcal{L}\psi_i^{(k)}, \psi_j^{(k)}] = \langle \mathcal{L}\psi_i^{(k)}, \psi_j^{(k)} \rangle_{L^2}$ ,  $B_{i,j}^{(k)} := [\mathcal{L}\chi_i^{(k)}, \chi_j^{(k)}] = \langle \mathcal{L}\chi_i^{(k)}, \chi_j^{(k)} \rangle_{L^2}$  are exponentially decaying as

$$A_{i,j}^{(k)} \leq C \exp \left( - \frac{\gamma \text{dist}(\tau_i^{(k)}, \tau_j^{(k)})}{h^k} \right),$$

$$B_{i,j}^{(k)} \leq C \exp \left( - \frac{\gamma \min \left\{ \text{dist}(\tau_i^{(k)}, \tau_{\tilde{i}}^{(k)}) | \tilde{i} \in \text{supp}(W_{i,\cdot}^{(k)}), \tilde{j} \in \text{supp}(W_{j,\cdot}^{(k)}) \right\}}{h^k} \right).$$

Furthermore Owhadi (2017, Theorem 4.17) shows that the matrices  $A^{(k)}$  and  $B^{(k)}$  have uniformly bounded condition numbers. Using these results Owhadi (2017) obtains an near linear time hierarchical algorithm for the nested computation of gamblets and for solving elliptic PDE with rough coefficients.

In Subsection 2.3 we have argued that the *screening effect* of conditioning translates to sparse Cholesky decompositions. Therefore it seems promising to use the estimates of Owhadi (2017) and Owhadi and Scovel (2017) to obtain sparse Cholesky decompositions of covariance matrices.

The  $\phi_i^{(k),\chi}$  define a multiresolution decomposition of  $\text{span} \{ \phi_i^{(q)} \}$ . It follows directly from the definition of the gamblets that for  $l > k$ :

$$\mathbb{E} \left[ [\phi_s^{(l),\chi}, u] | [\phi_j^{(k)}, u] = \delta_{i,j}, \forall j \right] = [\phi_s^{(l),\chi}, \psi_i^{(k)}].$$

Furthermore, basic linear algebra shows that

$$\text{Cov} \left[ [\phi_i^{(k),\chi}, u] [\phi_j^{(k),\chi}, u] | [\phi_s^{(k-1)}, u], \forall i, j \right] = (B^{(k)})^{-1}.$$

Define the matrices  $H^{(k)}$  by  $\phi_i^{(k),\chi} = \sum_j H_{i,j}^{(k)} \phi_j^{(q)}$  and the  $q \times 1$  block matrix  $(\mathcal{H}_{k,1})_{i,j} := H_{i,j}^k$ , for  $k \leq l$ . Let us for simplicity assume that the  $W$  and  $\pi$  are such that  $\mathcal{H}$  is an orthogonal matrix. Define the  $q \times q$  block matrix  $\Gamma$  as  $\Gamma_{i,j}^{k,l} := (H^{(k)} \Theta H^{(l),T})_{i,j}$ . We obtain the following algorithm:

---

**Algorithm 2:** Sparse block-factorisation via Gamblet transform.

---

**Data:** A covariance matrix  $\Theta$ , and a multiresolution basis  $\mathcal{H}$ .

**Result:** An exponentially localised triangular block matrix  $L$  and a blockdiagonal, exponentially localised matrix  $D$  such that the condition numbers of the blocks  $D_{k,k}$  are uniformly bounded, the exponentially localised lower triangular blockdiagonal Cholesky factor of  $D$ ,  $L^D$  such that  $\Theta = \mathcal{H}^T L D L^T \mathcal{H} = \mathcal{H}^T L L^D L^{D,T} L^T \mathcal{H}$ , and a matrix  $\Psi$  that contains in its columns a discretisation of the gamblets associated to the operator  $A$ .

Initialise  $L$  as a block-identity matrix (an identity matrix divided into blocks according to the levels  $\mathcal{H}$ ),  $D$  as a block-zero matrix (an all zero matrix divided into blocks according to the levels of  $\mathcal{H}$ );

$\Gamma \leftarrow \mathcal{H} \Theta \mathcal{H}^T$ ;

**for**  $k \leftarrow 1$  **to**  $q - 1$  **do**

$L_{k,k}^D \leftarrow \text{CHOL}(\Gamma_{k,k})$ ;

$L_{k+1:q,k} \leftarrow \Gamma_{k+1:q,k} \left( L_{k,k}^D L_{k,k}^{D,T} \right)^{-1}$  ;

$D_{k,k} \leftarrow \Gamma_{k,k}$  ;

$\Gamma_{k+1:q,k+1:q} \leftarrow \Gamma_{k+1:q,k+1:q} - \Gamma_{k+1:q,k} \left( L_{k,k}^D L_{k,k}^{D,T} \right)^{-1} \Gamma_{k,k+1:q}$ ;

$\Psi \leftarrow L \mathcal{H}$  ;

$L_{q,q}^D \leftarrow \text{CHOL}(\Gamma_{q,q})$  ;

$D_{q,q} \leftarrow \Gamma_{q,q}$

---

The estimates of Owhadi and Scovel (2017) show that, up to exponentially small entries, the matrices in the above algorithm will be sparse according to a pattern known a priori. Therefore a fast (near-linear complexity) version of Algorithm 2, similar to Algorithm 9, can be obtained by restricting the computation to the known sparsity patterns and the resulting factorisation allows for near-linear time inversion of  $\Theta$ . Furthermore, the columns of  $\Psi$  have the form  $\Psi_{i,j} = [\phi_i^{(q)}, \psi_j^{(k)}]$ , if the index  $j$  is part of the  $k$ -th level of the multiresolution basis. Hence, they contain a discretisation of the gamblets  $\psi_i^{(k)}$ . As mentioned in Owhadi and Scovel (2017) and exploited for low rank compression of operators in Hou and Zhang (2017), the gamblets provide an approximation of the principal components of the operator  $G$ . In particular, in Hou and Zhang (2017) it was conjectured that gamblets can also be computed directly from the covariance operator. Algorithm 2, with computation restricted to the near-sparsity patterns, provides a method for achieving this computation in near linear time based on and following the initial basis transformation. Algorithm 2 has nearly linear complexity if computation is reduced to the patterns of approximate sparsity of the gamblets, furthermore the relationship to the *gamblet transform* of Owhadi (2017) and Owhadi and Scovel (2017) is transparent. We will see in the next section that, analogously to the nested dissection, the decay estimates for gamblets also imply the sparsity of the hierarchical Cholesky decomposition. This leads to the following, simpler algorithm:

---

**Algorithm 3:** Zero fill-in Cholesky on  $S$  in multiresolution basis

---

**Data:** A covariance matrix  $\Theta \in \mathbb{R}^{I \times I}$ , a multiresolution basis  $\mathcal{H}$  (ordered from coarse to fine) and a set  $S \subset I \times I$

**Result:** A sparse lower triangular matrix  $L$  such that  $\Theta = \mathcal{H}^T L L^T \mathcal{H}$

Initialise  $\Gamma$  by  $\Gamma_{i,j} = \Theta_{i,j}$ , for  $(i,j) \in S$  and  $\Gamma_{i,j} = 0$ , else;

$\Gamma \leftarrow \mathcal{H} \Gamma \mathcal{H}^T$ ;

$L \leftarrow \text{ICHOL}(\Gamma, S)$  ;

---

Here,  $\text{ICHOL}(\Gamma, S)$  denotes the Cholesky factorisation, where every read or write operation involving entries of the complement of  $S$  is skipped, as described in Algorithm 6. Typically, if the size of the support of  $\phi_i^{(k),\chi}$  is of the order of  $h^k$ , then choosing the sparsity pattern  $S$  as

$$S_\rho := \left\{ (i, j) \mid i \in J^{(k)}, j \in J^{(l)}, \text{dist} \left( \text{supp} \left( \phi_i^{(k),\chi} \right), \text{supp} \left( \phi_j^{(l),\chi} \right) \right) \leq \rho h^{\min(k,l)} \right\}.$$

results in the exponential decay of the approximation error  $\|\Gamma - LL^T\|$  as a function of  $\rho$ . At this point, we can rigorously prove only the accuracy of the Block-Cholesky algorithm due to the lack of a suitable stability estimate of incomplete Cholesky decomposition. Numerically, however we very clearly observe the required stability, as discussed in Section 4.3.3.

Let  $i^{(k)}$  be, the last index on level  $k$  of the multiresolution basis. Then define the  $L^k := L_{:,1:i^{(k)}}$ . The operator  $L^{(k)}L^{(k),T}$ , then provides us with a low rank approximation of the operator  $\Theta$ , corresponding to the one obtained by projecting onto the space spanned by the gamblets  $\psi_i^{(k)}$ , at scale  $k$ . We note that if we only want the principal components of this approximate sparse PCA, we can simply stop the Cholesky decomposition prematurely. As in Algorithm 1, we only need compute those entries of  $\Gamma$  that lie on the sparsity pattern.

Although the complexity of the nested dissection algorithm deteriorates for  $d > 1$ , the proposed incomplete Cholesky decomposition remains of  $\mathcal{O}(N \text{polylog}(N))$  complexity in any spatial dimension  $d$  (with the order of the polylog depending on  $d$ ).

In Owhadi and Scovel (2017), the results of Owhadi (2017) were generalised to the abstract setting of bounded operators on Banach spaces (including arbitrary continuous linear bijections from  $H_0^s(\Omega)$  to  $H^{-s}(\Omega)$ ). Although the proof of exponential decay of gamblets provided in Owhadi and Scovel (2017) allows for very general measurement functions  $\phi_i^{(k)}$  (including masses of Diracs, indicator functions and higher order polynomials, see also Hou and Zhang (2017) for strongly elliptic PDEs with higher order polynomials as measurement functions), the proof Owhadi and Scovel (2017) that the matrices  $B^{(k)}$  have uniformly bounded condition numbers rely on vanishing moments of the underlying multiresolution basis. That is, they rely on the property that

$$\int_{\Omega_i^{(k)}} p \sum_{j \in I^{(q)}} \left( W^{(k)} \pi^{(k,q)} \right)_{i,j} \phi_j^{(q)} dx = 0$$

for all  $p \in \mathcal{P}_{2s-1}$  and for  $\text{diam}(\Omega_i^{(k)}) \approx h^k$ , if  $\Theta$  arises from the Green's function of an elliptic partial differential operator of order  $2s$ . This has a number of disadvantages:

1. The user, who might be given  $\Theta$  just in the form of a matrix, has to specify the estimated order of the differential operator a-priori. Furthermore, for unstructured grids, the construction of  $\pi$  and  $W$  might be complex.
2. The matrices  $H^{(k)}$  might need to have columns with many nonzero entries, corresponding to averages over large regions. While in the integral equations arising in numerical analysis it is usually possible to evaluate the Green's function at arbitrary points, allowing to use exponentially convergent quadrature formulae (Harbrecht and Schneider, 2006; Gantumur and Stevenson, 2006), this need not be the case in statistical applications, where unstructured grids are common. Therefore, the computation of the relevant entries of  $\Gamma$  to machine precision will typically not be possible in near-linear time.
3. The dependence on vanishing polynomials makes it more difficult to identify measurement functions on geometries other than  $\mathbb{R}^d$ .

## 2.5 A simple algorithm: subsampling, reordering and zero-fill in incomplete Cholesky decomposition

The explicit requirement that measurement functions have vanishing polynomial moments is an unnecessary limitation. We will, in Section 3.5.1, generalize the results of Owhadi and Scovel (2017) by relaxing

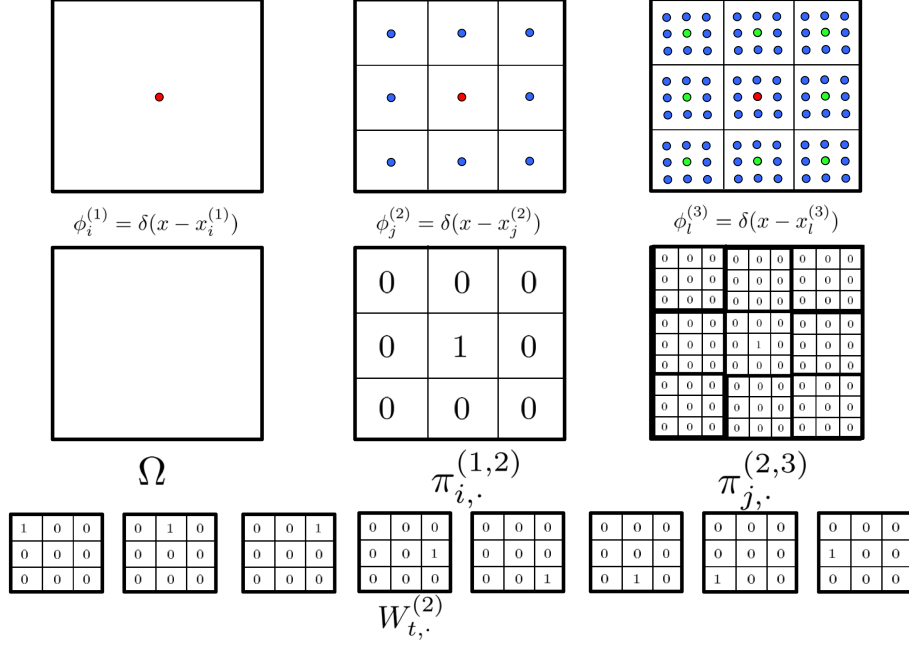


Figure 7: *Aggregation by Subsampling*: This figure, taken from Owhadi and Scovel (2017), shows the simple form that the  $\pi^{(k,l)}$  and  $W^{(k)}$  take under subsampling

the condition that measurement functions have vanishing polynomial moments used in Section 3.5.1 to show that the condition numbers of  $B^{(k)}$  are uniformly bounded. Under this generalization, the piecewise constant measurement functions of Owhadi (2017) can be proven to be sufficient for operators of arbitrary order. Furthermore, as a consequence of this generalization, in situations where pointwise measurements are defined (i.e., solutions are continuous), subsampling can be used as trivial aggregation scheme. If the grid spacing on the finest level is of order  $h^q$ , then coarse measurement functions on level  $k$  are then obtained from a subset of measurement functions with grid spacing of order  $h^k$ , as illustrated in Figure 7.

Therefore the basis transform  $\mathcal{H}$  in the above algorithm reduces to a permutation matrix and the orthogonalized gamblets are simply a subset of the original gamblets on the same level.

$$\left\{ \chi_i^{(k)} \right\}_{i \in J^{(k)}} = \left\{ \psi_i^{(k)} \right\}_{i \in I^{(k)}} \setminus \left\{ \psi_i^{(k-1)} \right\}_{i \in I^{(k-1)}}.$$

As in the introductory example of Section 1, if the  $\phi_i^{(q)}$  are localised around points  $\{x_i^{(q)}\}_{i \in I^q} \subset \Omega \subset \mathbb{R}^d$  with spacing  $\approx h^q$ , then we can split  $I := I^q$  into disjoint sets  $J^{(k)}$  for  $1 \leq k \leq q$  such that, for a constant  $\delta_{\text{mesh}}$ ,

$$\begin{aligned} \max_{x \in \Omega} \min_{j \in J^{(k)}} \text{dist}(x, x_j) &\leq h^{-k}, \\ \min_{i, j \in \cup_{1 \leq l \leq k} J^{(l)}} \text{dist}(x_i, x_j) &\geq \delta_{\text{mesh}} h^{-k}. \end{aligned}$$

Then,  $\mathcal{H}$  is simply given by the permutation matrix  $P$ , which orders the indices from  $J^{(1)}$  to  $J^{(q)}$ , with arbitrary ordering within each  $J^{(k)}$ . As in the introduction, we define

$$S_\rho := \left\{ (i, j) \text{ s. t. } i \in J^{(k)}, j \in J^{(l)}, \text{dist}(x_i, x_j) \leq \rho h^{\min(k, l)} \right\}.$$

Our algorithm is now straightforward:



---

**Algorithm 4:** Zero fill-in Cholesky on  $S$ , typically applied to and  $S$  similar to  $S_\rho$  as defined above; see Remark 2.2.

---

**Data:** A covariance matrix  $\Theta \in \mathbb{R}^{I \times I}$ , a permutation matrix  $P$  and a set  $S \subset I \times I$

**Result:** A sparse lower triangular matrix  $L$  such that  $\Theta = P^T L L^T P$

Initialise  $\Gamma$  by  $\Gamma_{i,j} = \Theta_{i,j}$ , for  $(i,j) \in S$  and  $\Gamma_{i,j} = 0$ , else;

$\Gamma \leftarrow P \Gamma P^T$ ;

$L \leftarrow \text{ICHOL}(\Gamma, S)$ ;

---

**Remark 2.2.** Algorithm 4 could be applied directly to  $S_\rho$ , but in order to easier keep track of the read- and write operations during the decomposition, it can be beneficial to extend  $S_\rho$  to a slightly larger set  $\tilde{S}_\rho$  that has a tree structure.

Here,  $\text{ICHOL}(\Gamma, S)$  is the Cholesky factorisation of  $\Gamma$  ignoring operations involving entries  $(i,j) \notin S$ . We note that, as before, we can obtain the first  $k$  components of an approximate sparse PCA of  $G$ , by stopping the Cholesky algorithm after  $k$  iterations.

## 2.6 Reordering revisited, and a simple algorithm for solving elliptic PDE with rough coefficients

Just as in our first approach to finding an ordering for the sparsifying Cholesky decomposition of the dense matrix  $\Theta$  turned out to be the reverse of the well known nested dissection ordering, the multiresolution ordering used in Algorithm 4 is reminiscent of the *minimum degree heuristic* of George and Liu (1989). The *minimum degree heuristic* consists in the elimination, at each step, of the remaining index with the lowest degree, according to the sparsity graph. After restricting  $\Theta$  to the hierarchical sparsity pattern used in Algorithms 2 and 4, our elimination ordering actually corresponds to a maximum, or reverse minimum degree ordering. The difference with the case of nested dissection, however, is that the graph by which we are choosing our maximum degree ordering is not the graph given by the nearest neighbour relations between the degrees of freedom. Once we have found this *hidden* graph according to which the maximum degree ordering leads to near-optimal results, we may again ask if we can invert the precision matrix using the reverse ordering. Indeed, just as in the case of the nested dissection ordering, one can show that the Cholesky decomposition of  $\Theta^{-1}$  is exponentially localised when performed in the minimum degree ordering according to  $S$ .

From the point of view of the numerical resolution of PDEs one usually starts with the precision operator  $\mathcal{L}$ . Using a Galerkin method (Braess, 2007; Bernardi et al., 2004), the equation

$$\mathcal{L}u = f$$

can be discretised by introducing a finite dimensional subspace  $V$  of the solution space  $\text{Im } \mathcal{L}^{-1}$ , and looking for  $u_V \in V$  such that

$$\langle v, \mathcal{L}u_\Phi \rangle_{L^2} = \langle v, f \rangle_{L^2} \quad \text{for all } v \in V.$$

This is just a finite dimensional system of linear equations which, picking a basis of  $V$ , can be written as

$$Ax = b.$$

If  $A^{-1}$  were a Gram matrix of the Green's function, then our results would immediately imply a near linear Cholesky factorisation of  $A$ . Since the results of Owhadi and Scovel (2017) hold for the discrete operator defined by the numerical discretization of  $\mathcal{L}$  (using a stable method), our incomplete Cholesky with a minimum degree ordering on  $S$  also provides a simple near-linear complexity algorithm for solving elliptic PDE with rough coefficients. Although the fine-to-coarse multiresolution Cholesky decomposition was suggested by Gines et al. (1998), their theoretical results relied on multiresolution bases with order  $p$  vanishing moments to achieve algebraic localisation of order  $p+1$ . In contrast, we can prove exponential decay without any need for vanishing moments. Again, we are lacking a sufficiently strong stability estimate for the incomplete Cholesky factorisation to prove rigorously the error estimates for the element-wise Cholesky factorisation. It seems as if such an estimate would also be required for the approach following Gines et al. (1998), but we could not find it in the literature.

### 3 Analysis of the Algorithm

#### 3.1 Setting and notation

In this subsection we present the abstract setting, in which we will prove the exponential decay of Cholesky decompositions. Let  $I^{(q)} := I$  be an index set and  $\Theta^{(q)} := \Theta \in \mathbb{R}^{I^{(q)} \times I^{(q)}}$  be a symmetric positive definite matrix. Assume that we are given families of index sets  $I^{(1)}, \dots, I^{(q-1)}$  and matrices  $\pi^{(k,l)} \in \mathbb{R}^{I^{(k)} \times I^{(l)}}$  such that  $\pi^{(k,l)} \pi^{(l,s)} = \pi^{(k,s)}$ ,  $\pi^{(k,l)} = \pi^{(l,k),T}$ , and  $\pi^{(k,k)} = \text{Id}_{I^{(k)}}$ . Let  $J^{(1)}, \dots, J^{(q)}$  and  $J := \bigcup_{1 \leq k \leq q} J^{(k)}$ , where we order the indices from  $J^1$  to  $J^q$  and let  $W^{(k)} \in \mathbb{R}^{J^{(k)} \times I^{(k)}}$ . Now define  $\Theta^{(k)} := \pi^{(k,q)} \Theta^{(q)} \pi^{(q,k)}$  and  $A^{(k)} := \Theta^{(k),-1}$ . Next, define for  $k \leq l$ :  $H^{(k,l)} := W^{(k)} \pi^{(k,l)}$  and

$$\mathcal{H}^{(k,l)} := \begin{pmatrix} H^{(1,l)} \\ \vdots \\ H^{(k,l)} \end{pmatrix}$$

and assume, that  $\mathcal{H}^{(k,k)}$  is an orthonormal matrix,  $\forall 1 \leq k \leq q$ . This can be guaranteed by assuming that  $\pi^{(l,k)} \pi^{(k,l)} = \text{Id}_{I^{(k)}}$  for  $l \leq k$  and  $W^{(k)} W^{(k),T} = \text{Id}_{J^{(k)}}$ , for all  $1 \leq k \leq q$ . Now we will define  $\Gamma^{(k)} := \mathcal{H}^{(k,q)} \Theta^{(q)} \mathcal{H}^{(k,q),T}$  and  $B^{(k)} := \Gamma^{(k),-1}$ . In the following we will use  $\Gamma := \Gamma^{(q)}$  to refer to the entire matrix in the multiresolution basis. Notice that it has  $J^{(m)}, J^{(l)}$ - blocks  $B_{l,m}^{(k)} H^{(l,k)} A^{(k)} H^{(k,m)}$ . In particular  $B_{k,k}^{(k)}$  is equal to the matrix  $B^{(k)}$  as in Owhadi (2017) and Owhadi and Scovel (2017). In the following, all block matrices  $M_{k,l}$  will be with respect to  $J^{(k)}, J^{(l)}$  and for such block matrices we will write  $M_{[r:s,n:m]}$  for the concatenation of the blocks  $M_{k,l}$  for  $k \in \{r, \dots, s\}$  and  $l \in \{n, \dots, m\}$ . The above notations will allow us to keep track of the order of averaging and inversion of the various submatrices appearing in our algorithm.

At this point we only assume  $\Theta$  to be positive definite. Over the course of this section we will prove the exponential decay of its Cholesky factors, by gradually introducing additional structure:

1. In Section 3.2, we will obtain a representation of a block-Cholesky decomposition of  $\Gamma = \Gamma^{(q)}$  based on its linear algebraic structure.
2. In Section 3.3, we introduce a notion of *hierarchical pseudodistance*, which assigns to each pair of indices in  $J \times J$  a notion of *distance*, adapted to the scale of the two indices. Using the fact that it fulfils a generalised triangle inequality, we can show that the Cholesky factors of  $\Gamma$  are exponentially decaying, under conditions on the exponential decay and condition numbers of submatrices forming the characterisation obtained in Section 3.2. Those conditions will be satisfied based on the properties of gamblets presented in Owhadi and Scovel (2017).
3. In Section 3.4, we prove the error- and complexity estimates for the incomplete Cholesky factorisation implied by the exponential decay of the Cholesky factors.
4. In Section 3.5 we extend the theory developed by Owhadi (2017) and Owhadi and Scovel (2017) to drop the requirement of vanishing moments in the proof of bounded condition numbers. We then use this theory to prove that the conditions identified in Section 3.3 are fulfilled for kernel matrices arising from appropriate measurement functionals of Green's functions associated to elliptic boundary value problems.
5. In Section 3.6, we put together the results of our previous section for three important classes of kernel matrices.
6. In Section 3.7, we comment on two byproducts of our theory and algorithm, notably the factorisation of precision matrices and the approximate sparse PCA.

#### 3.2 The Cholesky decomposition

In this subsection, we will, based on algebraic properties, formulate the block Cholesky decomposition in the basis given by the matrices  $\mathcal{H}^{(k,l)}$ . As a first step we consider only two scales:

**Lemma 3.1.** *With the notation from Section 3.1, for any  $1 \leq n \leq q$ , we have the following matrix identity:*

$$\Gamma^{(n)} = \begin{pmatrix} \Gamma_{[1:k],[1:k]}^{(n)} & \Gamma_{[1:k],[k+1:n]}^{(n)} \\ \Gamma_{[k+1:n],[1:k]}^{(n)} & \Gamma_{[k+1:n],[k+1:n]}^{(n)} \end{pmatrix} = LDL^T$$

with

$$L = \begin{pmatrix} \text{Id}_{J^{(1,k)}} & 0 \\ \Gamma_{[k+1:n],[1:k]}^{(n)} \left( \Gamma_{[1:k],[1:k]}^{(n)} \right)^{-1} & \text{Id}_{J^{(k+1,n)}} \end{pmatrix} = \begin{pmatrix} \text{Id}_{J^{(1,k)}} & 0 \\ \left( -B_{[k+1:n],[k+1:n]}^{(n)} \right)^{-1} B_{[k+1:n],[1:k]}^{(n)} & \text{Id}_{J^{(k+1,n)}} \end{pmatrix}$$

and

$$\begin{aligned} D &= \begin{pmatrix} \Gamma_{[1:k],[1:k]}^{(n)} & 0 \\ 0 & \Gamma_{[k+1:n],[k+1:n]}^{(n)} - \Gamma_{[k+1:n],[1:k]}^{(n)} \left( \Gamma_{[1:k],[1:k]}^{(n)} \right)^{-1} \Gamma_{[1:k],[k+1:n]}^{(n)} \end{pmatrix} \\ &= \begin{pmatrix} \Gamma_{[1:k],[1:k]}^{(n)} & 0 \\ 0 & \left( B_{[k+1:n],[k+1:n]}^{(n)} \right)^{-1} \end{pmatrix} \end{aligned}$$

*Proof.* The first equality for  $L$  and  $D$  is just the ordinary block Cholesky factorisation. For the second inequality, we define  $M_{1,1} := B_{[1:k],[1:k]}$ ,  $M_{1,2} := B_{[1:k],[k+1:n]}$ ,  $M_{2,1} := B_{[k+1:n],[1:k]}$  and  $M_{2,2} := B_{[k+1:n],[k+1:n]}$ . Now we can verify by simple matrix multiplication, that:

$$\begin{pmatrix} B_{1,1} & B_{1,2} \\ B_{2,1} & B_{2,2} \end{pmatrix} \begin{pmatrix} (B_{1,1} - B_{1,2} B_{2,2}^{-1} B_{2,1})^{-1} & -B_{1,1}^{-1} B_{1,2} (B_{2,2} - B_{2,1} B_{1,1}^{-1} B_{1,2})^{-1} \\ -B_{2,2}^{-1} B_{2,1} (B_{1,1} - B_{1,2} B_{2,2}^{-1} B_{2,1})^{-1} & (B_{2,2} - B_{2,1} B_{1,1}^{-1} B_{1,2})^{-1} \end{pmatrix} = \text{Id}$$

From this we can conclude

$$\Gamma^{(n)} = \begin{pmatrix} (B_{1,1} - B_{1,2} B_{2,2}^{-1} B_{2,1})^{-1} & -B_{1,1}^{-1} B_{1,2} (B_{2,2} - B_{2,1} B_{1,1}^{-1} B_{1,2})^{-1} \\ -B_{2,2}^{-1} B_{2,1} (B_{1,1} - B_{1,2} B_{2,2}^{-1} B_{2,1})^{-1} & (B_{2,2} - B_{2,1} B_{1,1}^{-1} B_{1,2})^{-1} \end{pmatrix}.$$

Plugging the above into the Schur complement we get the equation:

$$\begin{aligned} & \Gamma_{[k+1:n],[k+1:n]}^{(n)} - \Gamma_{[k+1:n],[1:k]}^{(n)} \left( \Gamma_{[1:k],[1:k]}^{(n)} \right)^{-1} \Gamma_{[1:k],[k+1:n]}^{(n)} \\ &= (B_{2,2} - B_{2,1} B_{1,1}^{-1} B_{1,2})^{-1} - B_{2,2}^{-1} B_{2,1} B_{1,1}^{-1} B_{1,2} (B_{2,2} - B_{2,1} B_{1,1}^{-1} B_{1,2})^{-1} \\ &= (B_{2,2} - B_{2,1} B_{1,1}^{-1} B_{1,2})^{-1} + B_{2,2}^{-1} (B_{2,2} - B_{2,1} B_{1,1}^{-1} B_{1,2}) (B_{2,2} - B_{2,1} B_{1,1}^{-1} B_{1,2})^{-1} \\ &\quad - B_{2,2}^{-1} B_{2,2} (B_{2,2} - B_{2,1} B_{1,1}^{-1} B_{1,2})^{-1} \\ &= B_{2,2}^{-1} = (B_{[k+1:n],[k+1:n]}^{(n)})^{-1}. \end{aligned}$$

This proves the characterisation of  $D$ , the second inequality for  $L$  by an analogous calculation.  $\square$

We remind the reader of the following well known quotient property of the Schur complement:

**Lemma 3.2** (Quotient property: Crabtree and Haynsworth (1969)). *Given a block matrix*

$$N := \begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

*Write its Schur complement with respect to the block  $A$  as*

$$(N/A) := D - CA^{-1}B.$$

*Then for a block matrix*

$$M := \begin{pmatrix} A & B & C \\ D & E & F \\ G & H & I, \end{pmatrix}$$

we have

$$\left( \left( \begin{pmatrix} A & B & C \\ D & E & F \\ G & H & I \end{pmatrix} / \begin{pmatrix} A & B \\ D & E \end{pmatrix} \right) = \left( \left( \left( \begin{pmatrix} A & B & C \\ D & E & F \\ G & H & I \end{pmatrix} / A \right) / \left( \begin{pmatrix} A & B \\ D & E \end{pmatrix} / A \right) \right)$$

**Remark 3.3.** In terms of jointly Gaussian vectors  $(X, Y, Z)$ , the quotient property simply states that

$$\text{Cov}[Z|X, Y] = \text{Cov}[(Z|X) | (Y|X)]$$

Now we can proceed to prove the following theorem:

**Theorem 3.4.** *We have the following decomposition:*

$$\Gamma^{(q)} = LDL^T$$

with  $L$  and  $D$  defined as:

$$D = \begin{pmatrix} B_{1,1}^{(1),-1} & 0 & \dots & \dots & 0 \\ 0 & B_{2,2}^{(2),-1} & \ddots & 0 & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & 0 & \ddots & B_{q-1,q-1}^{q-1,-1} & 0 \\ 0 & 0 & \dots & 0 & B_{q,q}^{(q),-1} \end{pmatrix},$$

and

$$L = \begin{pmatrix} \text{Id} & 0 & \dots & \dots & 0 \\ B_{2,2}^{(2),-1} B_{2,1}^{(2)} & \text{Id} & \ddots & 0 & \vdots \\ \vdots & B_{3,3}^{(3),-1} B_{3,2}^{(3)} & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \text{Id} & 0 \\ B_{q,q}^{(q),-1} B_{q,1}^{(3)} & B_{q,2}^{(q),-1} B_{q,2}^{(q)} & \dots & B_{q,q-1}^{(q),-1} B_{q,q-1}^{(q)} & \text{Id} \end{pmatrix}^{-1} = \begin{pmatrix} \text{Id} & 0 & \dots & \dots & 0 \\ L_{2,1} & \text{Id} & \ddots & 0 & \vdots \\ \vdots & L_{3,2} & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \text{Id} & 0 \\ L_{q,1} & L_{q,2} & \dots & L_{q,q-1} & \text{Id} \end{pmatrix},$$

where

$$L_{i,j} := \sum_{k=1}^j \Gamma_{i,k}^{(q)} B_{k,j}^{(j)} = \sum_{k=1}^j \Gamma_{i,k}^{(q)} \left( \Gamma^{(j),-1} \right)_{k,j}$$

This decomposition is in particular the one obtained by successive block-Cholesky factorisation of  $\Gamma^{(q)}$ .

*Proof.* Applying Lemma 3.1 to  $\Gamma^{(n)}$  with  $k = n - 1$  successively successively for  $n$  ranging from  $q$  to 2,

we obtain the following decomposition;

$$\begin{aligned}
& \begin{pmatrix} \Gamma_{1,1}^{(q)} & \cdots & \Gamma_{1,q-1}^{(q)} & \Gamma_{1,q}^{(q)} \\ \vdots & \ddots & \vdots & \vdots \\ \Gamma_{q-1,1}^{(q)} & \cdots & \Gamma_{q-1,q-1}^{(q)} & \Gamma_{2,q}^{(q)} \\ \Gamma_{q,1}^{(q)} & \cdots & \Gamma_{q,q-1}^{(q)} & \Gamma_{q,q}^{(q)} \end{pmatrix} \\
&= \begin{pmatrix} & & & 0 \\ & \text{Id} & & \vdots \\ & & & 0 \\ -B_{q,q}^{(q),-1} B_{q,1}^{(q)} & \cdots & -B_{q,q}^{(q),-1} B_{q,q-1}^{(q)} & \text{Id} \end{pmatrix} \begin{pmatrix} & & & 0 & 0 \\ & & \text{Id} & & \vdots \\ & & & & \vdots \\ -B_{q-1,q-1}^{(q-1),-1} B_{q-1,1}^{(q-1)} & \cdots & -B_{q-1,q-1}^{(q-1),-1} B_{q-1,q-2}^{(q-1)} & \text{Id} & 0 \\ 0 & \cdots & \cdots & 0 & \text{Id} \end{pmatrix} \cdots \\
&\cdots \begin{pmatrix} & & & & 0 \\ & \text{Id} & 0 & 0 & \\ -B_{2,2}^{(2),-1} B_{2,1}^{(2)} & \text{Id} & \vdots & & \\ 0 & \cdots & \text{Id} & & \end{pmatrix} \begin{pmatrix} B_{1,1}^{(1),-1} & 0 & \cdots & \cdots & 0 \\ 0 & B_{2,2}^{(2),-1} & \ddots & 0 & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & 0 & \ddots & B_{q-1,q-1}^{(q-1),-1} & 0 \\ 0 & 0 & \cdots & 0 & B_{q,q}^{(q),-1} \end{pmatrix} \begin{pmatrix} \text{Id} & -B_{1,2}^{(2)} B_{2,2}^{(2),-T} & 0 \\ 0 & \text{Id} & \vdots \\ 0 & \cdots & \text{Id} \end{pmatrix} \cdots \\
&\cdots \begin{pmatrix} & -B_{1,q-1}^{(q-1)} B_{q-1,q-1}^{(q-1),-T} & 0 \\ & \vdots & \vdots \\ \text{Id} & & \vdots \\ & -B_{1,q-1}^{(q-1)} B_{q-1,q-1}^{(q-1),-T} & \vdots \\ 0 & \cdots & 0 & \text{Id} & 0 \\ 0 & \cdots & \cdots & 0 & \text{Id} \end{pmatrix} \begin{pmatrix} & -B_{1,q}^{(q)} B_{q,q}^{(q),-T} \\ & \vdots \\ \text{Id} & & \\ & -B_{1,q}^{(q)} B_{q,q}^{(q),-T} \\ 0 & \cdots & 0 & \text{Id} \end{pmatrix}. \tag{3.1}
\end{aligned}$$

Now we want to characterise the triangular factors in the above equation. Using the well known characterisation of inverses of elementary triangular matrices, we obtain:

$$\begin{aligned}
& \begin{pmatrix} \text{Id} & B_{1,2}^{(2)} B_{2,2}^{(2),-T} & 0 \\ 0 & \text{Id} & \vdots \\ 0 & \cdots & \text{Id} \end{pmatrix} \cdots \begin{pmatrix} & B_{1,q-1}^{(q-1)} B_{q-1,q-1}^{(q-1),-T} & 0 \\ & \vdots & \vdots \\ 0 & \cdots & 0 & \text{Id} & 0 \\ 0 & \cdots & \cdots & 0 & \text{Id} \end{pmatrix} \begin{pmatrix} & B_{1,q}^{(q)} B_{q,q}^{(q),-T} \\ & \vdots \\ 0 & \cdots & 0 & \text{Id} \end{pmatrix} = \\
& \left( \begin{pmatrix} & B_{1,q}^{(q)} B_{q,q}^{(q),-T} \\ & \vdots \\ 0 & \cdots & 0 & \text{Id} \end{pmatrix} \begin{pmatrix} & B_{1,q-1}^{(q-1)} B_{q-1,q-1}^{(q-1),-T} & 0 \\ & \vdots & \vdots \\ 0 & \cdots & 0 & \text{Id} & 0 \\ 0 & \cdots & \cdots & 0 & \text{Id} \end{pmatrix} \cdots \begin{pmatrix} \text{Id} & B_{1,2}^{(2)} B_{2,2}^{(2),-T} & 0 \\ 0 & \text{Id} & \vdots \\ 0 & \cdots & \text{Id} \end{pmatrix} \right)^{-1} \\
&= \begin{pmatrix} \text{Id} & 0 & \cdots & \cdots & 0 \\ B_{2,2}^{(2),-1} B_{2,1}^{(2)} & \text{Id} & \ddots & 0 & \vdots \\ \vdots & B_{3,3}^{(3),-1} B_{3,2}^{(3)} & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \text{Id} & 0 \\ B_{q,q}^{(q),-1} B_{q,1}^{(q)} & B_{q,2}^{(q),-1} B_{q,2}^{(q)} & \cdots & B_{q,q-1}^{(q),-1} B_{q,q-1}^{(q)} & \text{Id} \end{pmatrix}^{-T} \tag{3.2}
\end{aligned}$$

This provides us with the first characterisation of the triangular factors of the decomposition. To obtain

the second factor, we calculate

$$LDL^T = \Gamma^{(q)} \iff L^T = D^{-1}L^{-1}\Gamma^{(q)}$$

from this follows the second characterisation of  $L$ . To show that this is the same factorisation that would be obtained by a block-Cholesky factorisation, we can deduce from the quotient property of Schur-complements, that the block-Cholesky factorisation leads to the same diagonal part. Since the Cholesky factorisation is unique, this shows that the factorisation obtained by the block-Cholesky algorithm is the same as the one we obtained above.  $\square$

### 3.3 Exponential decay

Up until now, we have only used the algebraic structure of the operator in order to find an alternative expression of its block-Cholesky decomposition in a given basis.

These expressions are useful because they provide a method for employing the decay estimates obtained in Owhadi (2017) and Owhadi and Scovel (2017) to prove that these matrices are nearly sparse. Most theories on the propagation of sparsity or exponential decay of matrices under operations like multiplication use the distance induced by the sparsity graph of the initial sparse matrix.

One difficulty that we have to deal with is that interactions between  $i, j \in J$  depends on the levels of the two indices. In particular, our notion of *distance* can not fulfill the triangle inequality, since the indices on the coarsest level are interacting with every other index. When modelling the kind of decay featured by gamblets, we can enforce the triangle inequality between indices  $i, j, s$  only if the coarsest level involved is one of the endpoints. This restricted triangle inequality turns out to be the right compromise to model the decay of gamblets, while still allowing to control its propagation under multiplication and inversion.

**Definition 3.5.** A function  $d: I^{(q)} \times I^{(q)} \longrightarrow \mathbb{R}$  is called a *hierarchical pseudometric* if

- (i)  $d(i, j) \geq 0$  for all  $i, j \in I^{(q)}$ ;
- (ii)  $d(i, i) = 0$  for all  $i \in I^{(q)}$ ;
- (iii)  $d(i, j) = d(j, i)$  for all  $i, j \in I^{(q)}$ ;
- (iv) for all  $1 \leq k \leq q$ , the restriction of  $d$  to  $J^{(k)} \times J^{(k)}$  is a metric;
- (v) for all  $1 \leq k \leq m, l \leq q$  and  $i_k \in I^{(k)}, j_l \in I^{(l)}, s_m \in I^{(m)}$ , we have  $d(i_k, j_l) \leq d(i_k, s_m) + d(s_m, j_l)$ .

The estimates in Owhadi (2017) and Owhadi and Scovel (2017), as generalised in the next section, imply that the following conditions hold true for a wide range of kernel matrices. We will for now take them for granted and elaborate on their scope in the next section.

**Condition 3.6** (Localised conditional expectations). We say that  $\Gamma$  has *localised conditional expectations* for constants  $C, \gamma$  with respect to the hierarchical pseudometric  $d$ , if, for all  $1 \leq k < l \leq q$  and  $i, j \in J$ ,

$$\left| \left( \Gamma_{[k+1:q], [1:k]}^q \Gamma^{(k), -1} \right)_{i,j} \right| \leq C \exp(-\gamma d(i, j)) \quad (3.3)$$

and for all  $1 \leq k \leq q$ :

$$\left| \left( \Gamma^{(k), -1} \right)_{i,j} \right| \leq C \exp(-\gamma d(i, j)) \quad (3.4)$$

**Condition 3.7** (Hierarchically bounded condition numbers). We say that  $\Gamma^{(q)}$  has *hierarchically uniformly bounded condition number* if there exists a  $\kappa > 0$  such that

$$\text{cond} \left( B_{k,k}^{(k)} \right) \leq \kappa, \quad \forall 1 \leq k \leq q.$$

We note that (3.3) immediately implies the exponential localisation of  $L$  as in Theorem 3.4 according to  $d$ .

**Lemma 3.8.** Assume  $\Gamma$  satisfies (3.3) with constants  $\gamma, C$ . Then we have

$$(L_{i,j}) \leq \tilde{C} \exp(-\gamma d(i,j))$$

where  $\tilde{C} := \max(1, C)$

*Proof.* We can show the result blockwise. Clearly, it holds true for the blocks on and above the diagonal. For the blocks below, we notice that

$$L_{k,l} := \sum_{m=1}^l \Gamma_{k,m}^{(q)} B_{m,l}^{(l)} = \left( \Gamma_{[1:q],[1:l]}^{(q)} \Gamma^{(l)-1} \right)_{k,l}$$

where the  $k$  and  $l$  are blocks, not entries. This is a submatrix of the matrix in equation (3.3), and hence has the desired decay.  $\square$

As a next step, we will want to show that the matrix  $D$  has a Cholesky decomposition that decays according to  $d$ . To this end, we will need to preserve the locality of  $B_{k,k}^{(k)}$  under inversion. There exist, in fact, a number of results saying roughly, that well conditioned localised matrices have localised inverses. These kinds of results have partly been phrased in a more abstract setting as the closedness of certain algebras (Jaffard, 1990; Krishtal et al., 2015), or more concretely providing non-asymptotic decay estimates (Demko et al., 1984). A general strategy by which those results are proven, is to use approximation theory to approximate the function  $x \mapsto x^{-1}$  by polynomials of order  $N$ , up to a term of order  $c^{-N}$ . Then, one can control the spread of the localisation when applying the polynomial to the original matrix. In the following we will need some very minor extensions of existing results of this kind.

First we need to find a way to control the localisation of the product of localised matrices. To this end, define:

$$c_{I,J,d}(\gamma) := \sup_{j \in J} \sum_{i \in I} \exp(-\gamma d(i,j))$$

and define  $c_{I,d} := c_{I,I,d}$ . We then need the following lemma (Jaffard, 1990), and which we only reprove for the sake of providing the constants.

**Lemma 3.9.** Let  $I_k$  be index sets for  $1 \leq k \leq n+1$  and let  $d: I_1 \cup \dots \cup I_n \times I_1 \cup \dots \cup I_n \rightarrow \mathbb{R}_{\geq 0}$  satisfy the following triangle-type inequality for  $i_k \in I_k$ :

$$d(i_1, i_{n+1}) \leq \sum_{k=1}^n d(i_k, i_{k+1})$$

Let  $A_k \in \mathbb{R}^{I_k \times I_{k+1}}$  for  $1 \leq k \leq n$  be such that  $|A_{i,j}| \leq C_k \exp(-\gamma d(i,j))$ . Then

$$\left( \prod_{k=1}^n A_k \right)_{i,j} \leq \left( \prod_{k=1}^n C_k \right) \left( \prod_{k=2}^n c_{I_k, I_{k+1}, d}(\gamma/2) \right) \exp\left(-\frac{\gamma}{2} d(i,j)\right).$$

*Proof.* Set  $i_1 := i, i_{n+1} := j$ . We then have

$$\begin{aligned} \left( \prod_{k=1}^n A_k \right)_{i,j} &\leq \left( \prod_{k=1}^n C_k \right) \sum_{i_2, \dots, i_n \in I} \exp\left(-\gamma \sum_{k=1}^n d(i_k, i_{k+1})\right) \\ &\leq \left( \prod_{k=1}^n C_k \right) \exp\left(-\frac{\gamma}{2} d(i_1, i_{n+1})\right) \sum_{i_2, \dots, i_n \in I} \exp\left(-\frac{\gamma}{2} \sum_{k=1}^n d(i_k, i_{k+1})\right) \\ &\leq \left( \prod_{k=1}^n C_k \right) \left( \prod_{k=2}^n c_{I_k, I_{k+1}, d}(\gamma/2) \right) \exp\left(-\frac{\gamma}{2} d(i,j)\right) \end{aligned} \quad (3.5)$$

$\square$



Now, we can proceed by proving the exponential decay of inverses by polynomial approximation of  $x \mapsto x^{-1}$ . Again, the proof is essentially taken from Jaffard (1990), we only keep track of constants. The results of Demko et al. (1984) are not immediately applicable since our matrices are not banded, but only exponentially localised.

**Lemma 3.10.** *For  $A \in \mathbb{R}^{I \times I}$  symmetric positive definite with  $A_{i,j} \leq C \exp(-\gamma d(i, j))$ , we have:*

$$\begin{aligned} (A^{-1})_{i,j} &\leq \frac{\|A\| + \|A^{-1}\|}{2} \exp\left(\frac{-2 \log(1-r)(1 + \log(c_{I,d}(\gamma/2)) + \log(C_k)) + \log(r) \frac{\gamma}{2} d(i, j)}{(1 + \log(c_{I,d}(\gamma/2)) + \log(C_k)) - \log(r)}\right) \\ &= \frac{\|A\| + \|A^{-1}\|}{2} \exp\left(\frac{-2 \log(1-r)(1 + \log(c_{I,d}(\gamma/2)) + \log(C_k))}{(1 + \log(c_{I,d}(\gamma/2)) + \log(C_k)) - \log(r)}\right) \\ &\quad \exp\left(\frac{\log(r)}{(1 + \log(c_{I,d}(\gamma/2)) + \log(C_k)) - \log(r)} \frac{\gamma}{2} d(i, j)\right) \\ &\leq \frac{\|A\| + \|A^{-1}\|}{2(1-r)^2} \exp\left(\frac{\log(r)}{(1 + \log(c_{I,d}(\gamma/2)) + \log(C_k)) - \log(r)} \frac{\gamma}{2} d(i, j)\right) \end{aligned} \quad (3.6)$$

where  $C_R := \max\left\{1, \frac{2C}{\|A\| + \|A^{-1}\|}\right\}$  and  $r := \frac{1 - \frac{\|A\|}{\|A^{-1}\|}}{1 + \frac{\|A\|}{\|A^{-1}\|}}$ .

*Proof.* Define  $R := \text{Id} - \frac{2}{\|A\| + \|A^{-1}\|} A$ . Then we have  $\|R\| \leq \frac{1 - \frac{\|A\|}{\|A^{-1}\|}}{1 + \frac{\|A\|}{\|A^{-1}\|}} =: r$ . Writing now:

$$A = \frac{2}{\|A\| + \|A^{-1}\|} (\text{Id} - R) \implies A^{-1} = \frac{\|A\| + \|A^{-1}\|}{2} \sum_{k=0}^{\infty} R^k$$

using positive definiteness of  $A$ , we obtain:

$$R_{i,j} \leq \max\left\{1, \frac{2C}{\|A\| + \|A^{-1}\|}\right\} \exp(-\gamma d(i, j))$$

Define  $C_R := \max\left\{1, \frac{2C}{\|A\| + \|A^{-1}\|}\right\}$ . Based on Lemma 3.9, we have

$$R_{i,j}^k \leq (c_{I,d}(\gamma/2))^{k-1} C_R^k \exp\left(-\frac{\gamma}{2} d(i, j)\right)$$

Combining the above estimates leads us to the estimate:

$$\begin{aligned} \frac{2}{\|A\| + \|A^{-1}\|} (A^{-1})_{i,j} &\leq (n+1) (c_{I,d}(\gamma/2))^{n-1} C_R^n \exp\left(-\frac{\gamma}{2} d(i, j)\right) + \frac{r^{n+1}}{1-r} \\ &\leq \exp\left((1 + \log(c_{I,d}(\gamma/2)) + \log(C_k))(n+1) - \frac{\gamma}{2} d(i, j)\right) \\ &\quad + \exp(-\log(1-r) + \log(r)(n+1)) \end{aligned} \quad (3.7)$$

If we want to balance the two terms, we would like to choose:

$$n+1 = \frac{\frac{\gamma}{2} d(i, j) - \log(1-r)}{(1 + \log(c_{I,d}(\gamma/2)) + \log(C_k)) - \log(r)},$$

yielding

$$\begin{aligned} &\exp\left((1 + \log(c_{I,d}(\gamma/2)) + \log(C_k))(n+1) - \frac{\gamma}{2} d(i, j)\right) \\ &\quad + \exp(-\log(1-r) + \log(r)(n+1)) \\ &= \exp\left(\frac{-\log(1-r)(1 + \log(c_{I,d}(\gamma/2)) + \log(C_k)) + \log(r) \frac{\gamma}{2} d(i, j)}{(1 + \log(c_{I,d}(\gamma/2)) + \log(C_k)) - \log(r)}\right) \end{aligned} \quad (3.8)$$

Since we have the constraint to choose  $n+1$  as an integer strictly bigger than 0, we have to increase  $n+1$  by up to a value smaller than one, compared to the above. This can be estimated by multiplying with another factor of  $-\log(1-r)(1 + \log(c_{I,d}(\gamma/2)) + \log(C_k))$ , leading to the first two inequalities of the result. By optimising over  $(1 + \log(c_{I,d}(\gamma/2)) + \log(C_k))$ , we obtain the result.  $\square$

With the above tools, we can now prove the exponential decay of the Cholesky factors of  $D$ . The following lemma appears in similar form in Benzi and Tũma (2000) for the case of banded matrices and in Krishtal et al. (2015), without explicit constants.

**Lemma 3.11.** *Let  $B \in \mathbb{R}^{I \times I} \simeq \mathbb{R}^{N \times N}$  be symmetric positive definite with  $B_{i,j} \leq C \exp(-\gamma d(i, j))$  for a pseudometric  $d$  on  $I$ . Then the Cholesky decomposition of its inverse  $(B)^{-1} = LL^T$  is such that*

$$L_{i,j} \leq \frac{\sqrt{\|B\|} (\|B\| + \|B^{-1}\|)}{2(1-r)^2} \exp\left(\frac{\log(r)}{(1 + \log(c_{I,d}(\gamma/2)) + \log(C_k)) - \log(r)} \frac{\gamma}{2} d(i, j)\right). \quad (3.9)$$

where  $C_R := \max\{1, 2C, \frac{2C}{\kappa}\}$  and  $r := \frac{1-\kappa}{1+\kappa}$ .

Results similar to the one above have already been used to prove the near-sparsity of well conditioned (near-)sparse matrices in Benzi and Tũma (2000) and Krishtal et al. (2015). The reason we provide a separate proof is that the first result is restricted to banded matrices and the second does not provide the constants of the decay.

*Proof.* We will show the result by looking showing that for all  $1 \leq k \leq N$ , the  $k^{\text{th}}$  column of  $L$  when considered as an element of  $\mathbb{R}^{I \times I}$  by zero padding, satisfies the exponential decay. Define,  $S^{(k)} := B_{k:n,k:n} - B_{k:n,1:k-1} (B_{1:k-1,1:k-1})^{-1} B_{1:k-1,k:n}$ . Then we have:  $L_{[k:N],k} = \frac{S_{[k],1}^{(k)}}{\sqrt{S_{k,k}^{(k)}}}$ . Using Lemma 3.1, we see that  $S^{(k)} = (B_{[k:n],[k:n]})^{-1}$  and hence by lemma 3.10, we have:

$$\begin{aligned} (S^{(k)})_{i,j} &\leq \frac{\|B\| + \|B^{-1}\|}{2} \exp\left(\frac{-\log(1-r)(1 + \log(c_{I,d}(\gamma/2)) + \log(C_k)) + \log(r)}{(1 + \log(c_{I,d}(\gamma/2)) + \log(C_k)) - \log(r)} \frac{\gamma}{2} d(i, j)\right) \\ &= \frac{\|B\| + \|B^{-1}\|}{2} \exp\left(\frac{-\log(1-r)(1 + \log(c_{I,d}(\gamma/2)) + \log(C_k))}{(1 + \log(c_{I,d}(\gamma/2)) + \log(C_k)) - \log(r)}\right) \\ &\quad \exp\left(\frac{\log(r)}{(1 + \log(c_{I,d}(\gamma/2)) + \log(C_k)) - \log(r)} \frac{\gamma}{2} d(i, j)\right). \end{aligned} \quad (3.10)$$

Here we made use of the fact that the spectrum of  $B_{k:n,k:n}$  is contained in the spectrum of  $B$ , that the maximal and minimal eigenvalue of  $B$  appear interchangeably or in the form of the condition number and that the right-hand side of the above estimate is increasing in  $r$  and  $C_R$ . Using the estimate  $S_{k,k}^{(k)} \geq \frac{1}{\|S^{(k),-1}\|} \geq \frac{1}{\|B\|}$ , we obtain the result.  $\square$

With the above preparation we can now show the near sparsity of the Cholesky decomposition of a near sparse matrix. For all Cholesky decopositions in the following, we use an elimination ordering  $\prec$  on  $J$ , such that for  $i \in J^{(k)}, j \in J^{(l)}$  and  $k < l$ , we have  $i \prec j$ .

**Theorem 3.12.** *Let  $\Gamma$  be fulfill Condition 3.6 with respect to the hierarchical pseudometric  $d$ , with constants  $\gamma, C$ , and let it fulfill Condition 3.7, with constant  $\kappa$ . Define furthermore  $C_R := \max\{1, 2C, \frac{2C}{\kappa}\}$  and  $r := \frac{1-\kappa}{1+\kappa}$  and:*

$$\tilde{C}_k := \frac{\sqrt{\|\Gamma^{-1}\|} (\|\Gamma\| + \|\Gamma^{-1}\|)}{2(1-r)^2}$$

and

$$\tilde{\gamma} = \frac{\log(r)}{(1 + \log(c_{I,d}(\gamma/2)) + \log(C_k)) - \log(r)} \frac{\gamma}{2}.$$

Then the matrix block  $D_{k,k}$  of the matrix  $D$  as in Theorem 3.4 has a Cholesky decomposition  $D_{k,k} = \tilde{L}^{(k)} \tilde{L}^{(k),T}$  such that

$$|\tilde{L}_{i,j}^{(k)}| \leq \tilde{C}_k \exp(-\tilde{\gamma} d(i, j))$$

And the element-wise Cholesky decomposition  $\Gamma = \bar{L} \bar{L}^T$  is localised as:

$$|\bar{L}_{i,j}| \leq \max_k \{c_{J^{(k)},d}(\tilde{\gamma}/2)\} C \exp(-\tilde{\gamma}/2 d(i, j))$$

*Proof.* The decay of  $D_{k,k}$  follows by applying Lemma 3.11 to the matrices  $B_{k,k}^{(k)}$ . The decay of  $\bar{L}$  follows then by writing the blocks  $\bar{L}_{k,l} = L_{k,l} \tilde{L}^{(l)}$ , where  $L_{k,l}$  is chosen as in Theorem 3.4 and applying Lemma 3.9.  $\square$

**Remark 3.13.** We point out, that the exponential decay of the Cholesky factors can be shown if in Condition 3.6, only exponential decay of the matrices  $A^{(k)}$  is provided. This can be done by looking at the characterisation of  $L$  as the inverse of a block- lower triangular matrix in Theorem 3.4. We notice, that this implies that  $L^{-1}$  is exponentially decaying. By writing  $L = \text{Id} + \sum_{k=1}^{\infty} (-1)^k L^{-k}$  as its Neumann series and noticing that this series converges after the first  $q$  elements because of the nilpotency of  $L^{-1} - \text{Id}$ , we can obtain the exponential decay of  $L$  using Lemma 3.9.

### 3.4 Computational complexity and error estimates

In the above section we have proven conditions, under which the Cholesky decomposition of a matrix is exponentially localised. While this is already enough to obtain a compression of the matrix by truncating the exponential tail of the entries, it is not a-priori sufficient to provide us with a linear algorithm. For the Cholesky-decomposition, however, sparsity of the resulting factorisation translates very naturally to low algorithmic complexity. We remind ourselves, that the algorithm for Cholesky decomposition is as follows:

---

**Algorithm 5:** Cholesky decomposition

---

**input** : A positive definite  $N \times N$  matrix  $\Theta$   
**output**: A lower triangular  $N \times N$  matrix  $L$ .

**for**  $i \leftarrow 1$  **to**  $N$  **do**  
    **for**  $j \leftarrow i$  **to**  $N$  **do**  
         $L_{i,j} \leftarrow \Theta_{i,j}$

**for**  $i \leftarrow 1$  **to**  $N$  **do**  
    **for**  $j \leftarrow i+1$  **to**  $N$  **do**  
         $L_{[j:N],j} \leftarrow L_{[j:N],j} - L_{[j:N],i} L_{j,i} / L_{i,i}$   
         $L_{i:N,i} \leftarrow L_{[i:N],i} / \sqrt{L_{i,i}}$

---

Assume now, that we want to restrict computation to a subset  $S \subset J \times J$ . Defining  $S_{\downarrow}(i) := \{(i,j) \in S \text{ s.t. } i \preceq j\}$ ,  $S_{\downarrow\downarrow}(i) := \{(i,j) \in S \text{ s.t. } i \prec j\}$ ,  $S_{\uparrow}(i) := \{(i,j) \in S \text{ s.t. } i \succeq j\}$ , and  $S_{\uparrow\uparrow}(i) := \{(i,j) \in S \text{ s.t. } i \succ j\}$ , we can compute the Cholesky decomposition restricted to  $S$ , as:

---

**Algorithm 6:** Cholesky decomposition restricted to  $S$

---

**input** : A positive definite  $N \times N$  matrix  $\Theta$  and a sparsity set  $S$   
**output**: A lower triangular  $N \times N$  matrix  $L$ , with support contained in  $S$

**for**  $i \leftarrow 1$  **to**  $N$  **do**  
    **for**  $j \in S_{\downarrow}(i)$  **do**  
         $L_{i,j} \leftarrow \Theta_{i,j}$

**for**  $i \leftarrow 1$  **to**  $N$  **do**  
    **for**  $j \in S_{\downarrow}(i)$  **do**  
         $L_{S_{\downarrow}(j) \cap S_{\downarrow}(i),j} \leftarrow L_{S_{\downarrow}(j),j} - L_{S_{\downarrow}(j) \cap S_{\downarrow}(i),i} L_{j,i} / L_{i,i}$   
         $L_{S_{\downarrow}(i),i} \leftarrow L_{S_{\downarrow}(i),i} / \sqrt{L_{i,i}}$

---

We first analyse the computational complexity of the algorithm.

**Lemma 3.14.** *The restricted Cholesky decomposition can be computed in  $\mathcal{O}(\#S) = \mathcal{O}\left(\sum_{i=1}^N \#S_{\downarrow}(i)\right) = \mathcal{O}\left(\sum_{i=1}^N \#S_{\uparrow}(i)\right)$  space- and  $\mathcal{O}\left(\sum_{i=1}^N \sum_{j \in S_{\downarrow}(i)} \#S_{\downarrow}(j)\right) = \mathcal{O}\left(\sum_{i=k}^N \sum_{j \in S_{\uparrow}(k)} \#S_{\uparrow}(j)\right)$  time complexity.*

*Proof.* The first equality can be read of directly from the pseudocode for Algorithm 6. For the second equality, we notice that the index  $(k,j)$  is updated during the line  $L_{S_{\downarrow}(i),i} \leftarrow L_{S_{\downarrow}(i),i} / \sqrt{L_{i,i}}$ , whenever  $j \in S_{\uparrow}(k)$ . Each such  $j$ , in turn, appears in the innermost loop whenever  $i \in S_{\uparrow}(j)$ .  $\square$

In order to apply the result to our Cholesky decomposition, we define for  $i \in J^{(k)}$  the *downward ball* of radius  $\rho$ :

$$B_{\rho,\downarrow}(i) := \{j \succ i \text{ s.t. } d(i, j) < \rho\}.$$

With this notation, the complexity of the incomplete Cholesky decomposition is easily described as follows:

**Corollary 3.15.** *The incomplete Cholesky decomposition as described in Theorem 3.12 has memory usage bounded above by  $\sum_{i \in J} \#B_{\rho,\downarrow}(i)$  and the number of read and write operations it needs to perform is bounded from above by  $\sum_{i \in J} \sum_{j \in B_{\rho,\downarrow}(i)} \#B_{\rho,\downarrow}(j)$ .*

*Proof.* The result follows since  $B_{\rho,\downarrow}(i) = S_{\downarrow}(i)$ , for  $S := \{i, j \text{ s.t. } d(i, j) \leq \rho\}$ .  $\square$

In order to bound this complexity, we need to make further assumptions regarding the size of the  $B_{\rho,\downarrow}(i)$ . A possible condition under which we obtain near-linear complexity is the following:

**Condition 3.16.** We say that  $J, d$  fulfill the low dimensionality condition if there exist  $C_d, d > 0$ , such that for all  $1 \leq k \leq q$ ,  $i \in J^{(k)}$  and  $\rho > 0$ , we have

$$\#J^{(k)} \cap B_{\rho,\downarrow}(i) \leq C_d \rho^d$$

**Condition 3.17.** We say that  $J, d$  fulfill the balance condition, if there exists a  $C > 0$ , such that for all  $1 \leq k \leq l \leq q$  and  $i \in J^{(k)}$ , we have

$$\#B_{0,\downarrow}(i) \cap J^{(l)} \leq C \frac{\#J^{(l)}}{\#J^{(k)}}$$

Under the above conditions, the complexity of the incomplete Cholesky decomposition is near linear:

**Theorem 3.18.** *Assume that  $J, d$  fulfill Conditions 3.16 and 3.17. The memory cost of the decomposition in Theorem 3.12 is bounded above by  $qCC_d\rho^d\#J$  and the number of read and write operations it performs is bounded by  $(qCC_d\rho^d)^2\#J$*

*Proof.* We notice, that for  $i \in J^{(k)}$ ,  $B_{\rho,\downarrow}(i) = \bigcup_{j \in J^{(k)} \cap B_{\rho,\downarrow}(i)} B_{0,\downarrow}(j)$ . Therefore, we have for  $i \in J^{(k)}$  and  $l \geq k$ :

$$\#J^{(l)} \cap B_{\rho,\downarrow}(i) \leq CC_d\rho^d \frac{\#J^{(l)}}{\#J^{(k)}}.$$

From this we conclude

$$\sum_{i \in J} \#B_{\rho,\downarrow}(i) = \sum_{k=1}^q \sum_{i \in J^{(k)}} \#B_{\rho,\downarrow}(i) \sum_{k=1}^q \sum_{i \in J^{(k)}} \#B_{\rho,\downarrow}(i) \leq \sum_{k=1}^q \sum_{i \in J^{(k)}} \sum_{l=k}^q \#(J^{(l)} \cap B_{\rho,\downarrow}(i)) \quad (3.11)$$

$$\leq \sum_{k=1}^q \sum_{i \in J^{(k)}} \sum_{l=k}^q CC_d\rho^d \frac{\#J^{(l)}}{\#J^{(k)}} \leq \sum_{k=1}^q \sum_{i \in J^{(k)}} CC_d\rho^d \frac{\#J}{\#J^{(k)}} = qCC_d\rho^d\#J \quad (3.12)$$

By applying the above argument twice, we obtain the bound on the time complexity:

$$\sum_{i \in J} \sum_{j \in \#B_{\rho,\downarrow}(i)} \#B_{\rho,\downarrow}(j) = \sum_{k=1}^q \sum_{i \in J^{(k)}} \sum_{l=k+1}^q \sum_{j \in \#B_{\rho,\downarrow}(i) \cap J^{(l)}} \#B_{\rho,\downarrow}(j) \quad (3.13)$$

$$= \sum_{k=1}^q \sum_{i \in J^{(k)}} \sum_{l=k}^q \sum_{j \in \#B_{\rho,\downarrow}(i) \cap J^{(l)}} \sum_{r=l}^q \#(B_{\rho,\downarrow} \cap J^{(r)})(j) \quad (3.14)$$

$$\leq \sum_{k=1}^q \sum_{i \in J^{(k)}} \sum_{l=k}^q \sum_{j \in \#B_{\rho,\downarrow}(i) \cap J^{(l)}} \sum_{r=l}^q qCC_d\rho^d \frac{\#J^{(r)}}{\#J^{(l)}} \quad (3.15)$$

$$\leq \sum_{k=1}^q \sum_{i \in J^{(k)}} \sum_{l=k}^q \sum_{r=l}^q CC_d\rho^d \frac{\#J^{(r)}}{\#J^{(k)}} \leq \sum_{k=1}^q \sum_{l=k}^q \sum_{r=l}^q CC_d\rho^d \#J^{(r)} \leq q^2 CC_d\rho^d \#J \quad (3.16)$$

$\square$

**Remark 3.19.** We point out that the above theorem does not treat the question of how to trace the sparsity pattern during the algorithm. This can however be done using standard tree-like constructions and we will comment more on this topic in the next section

Unfortunately despite the exponential decay of the Cholesky factors and good numerical results, we were not able to provide accuracy estimates for the incomplete Cholesky factorisation as described in Algorithm 6. For a given  $\Theta^{(q)}$  satisfying the requirements for exponential decay, for a given  $\rho$ , there exist perturbations  $E$  with  $|E| \leq N^\alpha \exp(-\gamma\rho)$  for  $\alpha, \gamma$  independent of  $N$  such that incomplete Cholesky decomposition with sparsity set  $S_\rho$  applied to  $\Theta^{(q)} + E$  is exactly accurate. The stability analysis of incomplete Cholesky decomposition, however, is more intricate than the corresponding analysis of ordinary Cholesky decomposition, since the former does not have the simple closed form expression in terms of Schur complements. Therefore, in order to prove the existence of a near linear algorithm that is provably correct, we will introduce the block version of the Cholesky factorisation. We start out by showing that a sparse approximation of the exponentially decaying Cholesky factor of a well-conditioned sparse matrix can be obtained in near-linear time.

**Lemma 3.20.** *Let  $A \in \mathbb{R}^{I \times I}$  be a matrix such that  $d(i, j) > \rho$ , for some  $\rho > 0$  and a metric  $d(\cdot, \cdot)$  on  $I \times I$  that fulfills Condition 3.16 with constants  $C_d, d$ . Assume furthermore, that  $\text{cond}(A) \leq \kappa$ . Then it is possible to compute any element  $A_{i,j}^{-1}$  in time complexity  $C_d^2 (\tau\rho + 1)^d (\rho + 1)^d \tau$ , where*

$$\tau = \frac{-\log(\epsilon) + \log(2) + \log(\kappa)}{\log\left(\frac{\sqrt{\kappa}+1}{\sqrt{\kappa}-1}\right)} + 1, \quad (3.17)$$

with an approximation error  $|A_{i,j} - \tilde{A}_{i,j}^{-1}| \leq \epsilon$ .

*Proof.* The computation can be done by using the conjugate gradient algorithm (Shewchuk et al., 1994) to apply the inverse of  $A$  to  $e_i$ . Setting *zero* as a starting point, we notice, that the first  $\tau - 1$  iterations of the conjugate gradient algorithm will be localised to  $\{i \in I \text{ s.t. } d(i, j) \leq \rho\tau\}$ . Therefore, if we choose to only perform those first  $\tau - 1$  steps, we don't ever have to update the other values of the iterate. This fact, together with the exponential convergence of conjugate gradient for well conditioned matrices yields the result.  $\square$

**Corollary 3.21.** *For Matrix  $A$  as in the above theorem and a sparsity pattern  $S \subset S_\rho$ , we can compute  $(A^{-1})|_S$  with error  $\epsilon$  in  $\|\cdot\|_\infty$  in time complexity  $C_d^2 (\tau\rho + 1)^d (\rho + 1)^d \tau \#S$*

Formally, this algorithm can be written as:

---

**Algorithm 7:** Matrix inversion restricted to  $S$  by element-wise computation .

---

**input** : A matrix  $A$  with known bandwidth  $\rho$  with respect to the distance  $d$ , an accuracy parameter  $\tau$  and a sparsity set  $S$

**output:** An approximation  $B$  of  $A^{-1}$ , with support contained in  $S$

**for**  $i \leftarrow 1$  **to**  $N$  **do**

**for**  $j \in S_\downarrow(i)$  **do**  
         $B_{i,j} \leftarrow A_{i,j}^{-1}$ , using  $\tau$  steps of gradient descent.

---

We denote the above algorithm as  $\text{EINV}(A, \rho, \tau, S, d)$ .

**Lemma 3.22.** *Let  $A$  be as in Lemma 3.20 Let, for any  $1 \leq k \leq n := \#I$ , be  $S := A_{k+1:n, k+1:n} / A_{1:k, 1:k}$  be the Schur complement of  $A_{1:k, 1:k}$  in  $A_{k+1:n, k+1:n}$ . Then it is possible to compute an approximation  $\tilde{S}_{i,j}$  of any element  $S_{i,j}$  in time complexity  $C_d^2 (\tau\rho + 1)^d (\rho + 1)^d \tau$ , where*

$$\tau = \frac{-\log(\epsilon) + \log(2) + \log(\kappa)}{\log\left(\frac{\sqrt{\kappa}+1}{\sqrt{\kappa}-1}\right)} + 1, \quad (3.18)$$

and up to an accuracy  $|\tilde{S}_{i,j} - S_{i,j}| \leq 2\epsilon \|A^{-1}\|^2$  for any  $\epsilon < \lambda_{\min}/2$ .

*Proof.* The computation can be done from the definition of the Schur-complement:

$$S_{i,j} := A_{i,j} - A_{i,1:k} (A_{1:k,1:k})^{-1} A_{1:k,j}, \quad (3.19)$$

by using the conjugate gradient algorithm (Shewchuk et al., 1994) to apply the inverse of  $A_{1:k,1:k}$ . Setting *zero* as a starting point, we notice, that the first  $\tau - 1$  iterations of the conjugate gradient algorithm will be localised to  $\{i \in I \text{ s.t. } d(i, j) \leq \rho\tau\}$ . Therefore, if we choose to only perform those first  $\tau - 1$  steps, we don't ever have to update the other values of the iterate. This fact, together with the exponential convergence of conjugate gradient for well conditioned matrices yields the result.  $\square$

Since the factors of the Cholesky decomposition of such a matrix are expressible in terms of the Schur complements, we thus can also evaluate them, entry wise.

**Corollary 3.23.** *Under the same conditions as in the last theorem,  $\epsilon \leq \lambda_{\min}(A)/2$ , we can compute arbitrary entries of the Cholesky factors of  $A$  with an error bounded by*

$$|L_{i,j} - \tilde{L}_{i,j}| \leq 4\epsilon \frac{4\lambda_{\max}(A)}{(\lambda_{\min})^{7/2}} \quad (3.20)$$

in time complexity  $2C_d^2(\tau\rho + 1)^d(\rho + 1)^d\tau$

The above results provide us with an efficient and provably accurate way to compute approximate the Cholesky factors a banded, well conditioned matrix:

---

**Algorithm 8:** Cholesky decomposition restricted to  $S$  by element-wise computation.

---

**input** : A matrix  $A$  with known bandwidth  $\rho$  with respect to the distance  $d$ , an accuracy parameter  $\tau$  and a sparsity set  $S$

**output:** A lower triangular  $N \times N$  matrix  $L$ , with support contained in  $S$

**for**  $i \leftarrow 1$  to  $N$  **do**

**for**  $j \in S_{\downarrow}(i)$  **do**

$a = (A_{i:n,i:n}/A_{1:i-1,1:i-1})_{i,i}$ , using  $\tau$  steps of conjugate gradient descent;

$b = (A_{i:n,i:n}/A_{1:i-1,1:i-1})_{i,j}$ , using  $\tau$  steps of conjugate gradient descent;

$L_{i,j} \leftarrow \frac{b}{\sqrt{a}};$

---

We denote the above algorithm as  $\text{EICHOL}(A, \rho, \tau, S, d)$ .

**Lemma 3.24.** *Algorithm  $\text{EICHOL}(A, \tau, S, d)$  has space complexity  $\max(\#S, \#I)$  and time complexity  $C_d^2(\tau\rho + 1)^d(\rho + 1)^d\tau\#S$ .*

---

**Algorithm 9:** Blockwise computation of Cholesky decomposition restricted to  $S$  by element-wise computation.

---

**input** : A block matrix  $q$  times  $q$   $\Gamma$ , a distance function  $d$  on its index set, an accuracy parameter  $\tau$  and a sparsity set  $S$  s.t.  $S \subset S_\rho$

**output:** A lower triangular block matrix  $L$ , with support contained in  $S$

**for**  $k \leftarrow 1$  to  $q$  **do**

**for**  $l \leftarrow k + 1$  to  $N$  **do**

$L_{k,l}|_S \leftarrow \Gamma_{k,l}|_S$

**for**  $k \leftarrow 1$  to  $q$  **do**

$T \leftarrow \text{EINV}(L_{k,k}, \rho, \tau, S, d);$

$L_{k,k} \leftarrow \text{EICHOL}(L_{k,k}, \rho, \tau, S, d);$

**for**  $l \leftarrow k + 1$  to  $q$  **do**

$L_{l,k}|_S \leftarrow (L_{l,k}T L_{k,k})|_S;$

**for**  $m \leftarrow k + 1 : l$  **do**

$L_{l,m}|_S \leftarrow L_{l,m}|_S - \left( L_{l,k} (L_{m,k})^T \right)|_S;$

We note that in the line  $L_{l,k}|_S \leftarrow (L_{l,k}TL_{k,k})|_S$  in the above is approximately equivalent to  $L_{l,k}|_S \leftarrow (L_{l,k}TL_{k,k})|_S$ . The reason for this somewhat indirect way to compute it is that the error propagation of forward substitution restricted to a sparsity pattern is, surprisingly difficult, just as the control of the error propagation in incomplete Cholesky decomposition, and this (theoretical) complication can be avoided by the above computation. With this in mind, the above algorithm obtains a Cholesky decomposition of the entire matrix, by performing an ordinary Cholesky decomposition of the level of the blocks, replacing the square root by EICHOL. We proceed by first proving a bound on its runtime:

**Theorem 3.25.** *Assume that  $J$  and  $d$  fulfill Conditions 3.16 and 3.17 with constants  $d, C_d$  and  $C$ . Then the space complexity of Algorithm 9 is bounded from above by  $qCC_d\rho^d\#J$  and the time-complexity is bounded by*

$$(qCC_d\rho^d)^2\#J + qCC_d^3\rho^{3d}\#J + C_d^2(\tau\rho + 1)^d(\rho + 1)^d\tau qCC_d\rho^d\#J \quad (3.21)$$

*Proof.* The space complexity is the same as the one of Algorithm 6 since both algorithms use the same sparsity pattern. For the time-complexity, we first note that the runtime produced by the calls to EICHOL and EINV can be bounded from above by  $C_d^2(\tau\rho + 1)^d(\rho + 1)^d\tau\#S$ . Using the bound  $\#S \leq qCC_d\rho^d\#J$  from the memory complexity we can bound this above by:

$$C_d^2(\tau\rho + 1)^d(\rho + 1)^d\tau qCC_d\rho^d\#J \quad (3.22)$$

Now for the runtime of the line

$$L_{l,k}|_S \leftarrow (L_{l,k}TL_{k,k})|_S, \quad (3.23)$$

we note that the number of entries matrix entries that need to be computed is given by

$$\sum_{i \in J^{(k)}} \#(B_{\rho,\downarrow}(i) \cap J^{(l)}) \quad (3.24)$$

The inner two inner loops of the matrix multiply each go over  $C_d\rho^d$  components, leaving us with complexity

$$C_d^2\rho^{2d} \sum_{i \in J^{(k)}} \#(B_{\rho,\downarrow}(i) \cap J^{(l)}). \quad (3.25)$$

Summing the above over all  $l$  and  $k$ , we obtain from this as an upper bound:

$$C_d^2\rho^{2d} \sum_{i \in J} \sum \#(B_{\rho,\downarrow}(i)). \quad (3.26)$$

Just as in Theorem 3.18, this can be bounded by

$$qCC_d^3\rho^{3d}\#J. \quad (3.27)$$

Next we adress the complexity produced by the line

$$L_{l,m}|_S \leftarrow L_{l,m}|_S - \left( L_{l,k}(L_{m,k})^T \right)|_S \quad (3.28)$$

For a given  $k < m \leq l$ , the complexity incurred of this is bounded from above by

$$\sum_{i \in J^{(k)}} \sum_{j \in B_{\rho,\downarrow}(i) \cap J^{(m)}} \#(B_{\rho,\downarrow}(j) \cap J^{(l)}). \quad (3.29)$$

Summing over all  $k, l, m$ , we get as an upper bound for the time complexity:

$$\sum_{i \in J} \sum_{j \in B_{\rho,\downarrow}(i)} \#B_{\rho,\downarrow}(j). \quad (3.30)$$

which we bounded in the proof of Theorem 3.18 from above by:

$$(qCC_d\rho^d)^2\#J. \quad (3.31)$$

□



Next, we want to prove a bound on the approximation error of Algorithm 9. First we introduce the following notation:

**Definition 3.26.** Let  $M \in \mathbb{R}^{J \times J}$  be a symmetric matrix, which we consider as a  $q \times q$  block matrix according to the  $J^{(1)} \dots J^{(q)}$ . For a  $1 \leq k \leq q$ , let the block  $M_{l,m}$  be zero for all  $(m, l)$  such that  $\min(m, l) < k$  and let  $M_{k:q, k:q}$  be strictly positive definite. We then define the Schur complement operator  $\mathbb{S} : \mathbb{R}^{J \times J} \longrightarrow \mathbb{R}^{J \times J}$  as:

$$\mathbb{S}(M) := M - M_{1:q, k} (M_{k, k})^{-1} M_{k, 1:q}, \quad (3.32)$$

That is,  $\mathbb{S}$  corresponds to one outer iteration step of exact block-Cholesky factorisation. We next define the approximate block-Cholesky operator  $\tilde{\mathbb{S}}$  as the remaining  $k+1 : q \times k+1 : q$  block matrix after an iteration of Algorithm 9, padded with zeros to a  $1 : q \times 1 : q$  block matrix and extended symmetrically.

With the above definition, the remaining matrix after  $k$  outer iterations of exact block-Cholesky decomposition applied to  $M$  can be obtained as  $\mathbb{S}^k(M)$ , and the remaining matrix after  $k$  outer iterations of Algorithm 9 is equal to  $\tilde{\mathbb{S}}^k(M)$ . As we apply more and more iterations of  $\mathbb{S}$  and  $\tilde{\mathbb{S}}$ , respectively, we expect the results to diverge from each other. In the following, we want obtain a bound on the speed, with which this error amplifies. In order to do so, we first need to obtain an error bound for EINV:

**Lemma 3.27.** Assume that  $A, \mathcal{E} \in \mathbb{R}^{J^{(k)} \times J^{(k)}}$  are matrices such that  $0 < \lambda_{\min} \leq \lambda_{\min}(A) \leq \lambda_{\max}(A) \leq \lambda_{\max}$ ,  $\kappa(A) \leq \kappa$  and  $\|E\|_{\text{Fro}} \leq \mathcal{E} < \lambda_{\min}/4$ . Assume, we have the exponential decay according to a metric  $d$ :

$$|A_{i,j}|, |A_{i,j}^{-1}| \leq C_\gamma \exp(-\gamma d(i, j)). \quad (3.33)$$

Let  $S$  be a sparsity set such that  $S_{\rho_{\min}} \subset S \subset S_{\rho_{\max}}$ . We then have:

$$\left\| (A + E)^{-1} - \text{EINV}(A, \rho_{\max}, \tau, S, d) \right\| \leq \left( \frac{2}{\lambda_{\min}^2} + 1 \right) \left( \#J^{(k)} \right)^2 C_\gamma \exp(-\gamma \rho_{\min}) + \frac{2}{\lambda_{\min}^2} \mathcal{E} + \left( \#J^{(k)} \right)^2 \epsilon_\tau, \quad (3.34)$$

where  $\epsilon_\tau$  is the error made during the element-wise computation of the inverse, due to the early stopping of the conjugate gradient algorithm.

*Proof.* We notice by applying the triangle inequality, and the estimate

$$\left\| (A + E)^{-1} - A^{-1} \right\| = \left\| (A - E)^{-1} E A^{-1} \right\| \leq \frac{2}{\lambda_{\min}^2}, \quad (3.35)$$

for  $\|E\| \leq \lambda_{\min}/4$ , we obtain:

$$\begin{aligned} & \left\| (A + E)^{-1} - \text{EINV}((A + E)|_S, \rho_{\max}, \tau, S, d) \right\| \\ & \leq \left\| (A + E)^{-1} - ((A + E)|_S)^{-1} \right\| + \left\| (A + E)^{-1} - A^{-1} \right\| \\ & \quad + \left( \#J^{(k)} \right)^2 \epsilon_\tau + \left( \#J^{(k)} \right)^2 C_\gamma \exp(-\gamma \rho_{\min}) \\ & \leq \left( \frac{2}{\lambda_{\min}^2} + 1 \right) \left( \#J^{(k)} \right)^2 C_\gamma \exp(-\gamma \rho_{\min}) + \frac{2}{\lambda_{\min}^2} \mathcal{E} + \left( \#J^{(k)} \right)^2 \epsilon_\tau \end{aligned} \quad (3.36)$$

□

**Lemma 3.28.** For  $1 \leq k \leq q$  let  $M$  be a  $q \times q$  block matrix, such that the  $M_{m,l} = 0$  for  $\min(m, l) < k$ ,  $0 < \lambda_{\min} \leq \lambda_{\min}(M_{k:q, k:q}) \leq \lambda_{\max}(M_{k:q, k:q}) \leq \lambda_{\max}$  and  $\kappa(M) \leq \kappa$ . Let  $S$  be a sparsity set such that  $S_{\rho_{\min}} \subset S \subset S_{\rho_{\max}}$ . Assume, that  $\|M_{k,:}\|_{\text{Fro}} \leq \epsilon/2$  and let  $E \in \mathbb{R}^{J \times J}$  be such that  $\|E\|_{\text{Fro}} \leq \mathcal{E} < \lambda_{\min}/4$ . and furthermore assume that  $A_{i,j}, A_{i,j}^{-1}, \mathbb{S}(A)_{i,j} \leq C_\gamma \exp(-\gamma d(i, j))$ . Then we have:

$$\left\| \mathbb{S}(M + E) - \tilde{\mathbb{S}}(M + E) \right\|_{\text{Fro}} \quad (3.37)$$

$$\leq N^2 \left( 4 (\mathcal{E} + \mathcal{E}^2) (\lambda_{\max} + \lambda_{\max}^2) \left( \left( \frac{2}{\lambda_{\min}^2} + 1 \right) \left( \#J^{(k)} \right)^2 C_\gamma \exp(-\gamma \rho_{\min}) + \frac{2}{\lambda_{\min}^2} \mathcal{E} + \left( \#J^{(k)} \right)^2 \epsilon_\tau \right) \right. \quad (3.38)$$

$$\left. + 32 (\mathcal{E} + \mathcal{E}^2) (\lambda_{\max} + \lambda_{\max}^2) \left( \left( \frac{2}{\lambda_{\min}^2} + 1 \right) \right) + 4\kappa^2 \lambda_{\max} n^2 C_\gamma \exp(-\gamma \rho_{\min}) \right) \quad (3.39)$$

$$\leq F(\lambda_{\min} \lambda_{\max}, N, C_\gamma) ((\mathcal{E} + \mathcal{E}^2) + \epsilon_{\rho_{\min}} + \epsilon_\tau) \quad (3.40)$$

For

$$F(\lambda_{\min}, \lambda_{\max}, N, C_\gamma) = CN^2 (1 + C_\gamma) (\lambda_{\max} + \lambda_{\max}^2 + \lambda_{\min}^{-1} + \lambda_{\min}^{-2}), \quad (3.41)$$

with  $C$  an absolute constant and  $\epsilon_{\rho_{\min}} = \exp(-\gamma \rho_{\min})$ .

*Proof.* We begin by introducing the notation  $A := M_{k,k}$ ,  $B := M_{k+1:q,k}$  and  $C := M_{k+1:q,k+1:q}$ . By abuse of notation, we will write  $A + E = A + E_{k,k}$ ,  $B + E = B + E_{k+1:q,k}$  and  $C + E = C + E_{k+1:q,k+1:q}$ . Now we compute:

$$\begin{aligned} & \left\| \tilde{\mathbb{S}}(M) - \tilde{\mathbb{S}}(M) \right\| \\ & \leq \left\| \left( (B + E)|_S \text{EINV}(A, \rho_{\max}, \tau, S, d) (B + E)^T |_S \right) \Big|_S - (B + E)(A + E)^{-1}(B + E)^T \right\| \\ & \leq \left\| (B + E)|_S (A + E)^{-1} (B + E)^T |_S - (B + E)(A + E)^{-1}(B + E)^T \right\| \\ & \quad + \left\| (B + E)|_S (A + E)^{-1} (B + E)^T |_S - \left( (B + E)|_S (A + E)^{-1} (B + E)^T |_S \right) \Big|_S \right\| \\ & \quad + \left\| \left( (B + E)|_S \text{EINV}((A + E)|_S, \rho_{\max}, \tau, S, d) (B + E)^T \Big|_S \right) \Big|_S - \left( (B + E)|_S (A + E)^{-1} (B + E)^T \Big|_S \right) \Big|_S \right\| \end{aligned} \quad (3.42)$$

The last term of the above right hand side can be estimated by Lemma 3.27 to be:

$$\begin{aligned} & \left\| \left( (B + E)|_S \text{EINV}((A + E)|_S, \rho_{\max}, \tau, S, d) (B + E)^T \Big|_S \right) \Big|_S - \left( (B + E)|_S (A + E)^{-1} (B + E)^T \Big|_S \right) \Big|_S \right\| \\ & \leq 4 (\mathcal{E} + \mathcal{E}^2) (\lambda_{\max} + \lambda_{\max}^2) \left( \left( \frac{2}{\lambda_{\min}^2} + 1 \right) \left( \#J^{(k)} \right)^2 C_\gamma \exp(-\gamma \rho_{\min}) + \frac{2}{\lambda_{\min}^2} \mathcal{E} + \left( \#J^{(k)} \right)^2 \epsilon_\tau \right), \end{aligned} \quad (3.43)$$

For the first and second term, using the linearity of the truncation operation, we get

$$\left\| (B + E)|_S (A + E)^{-1} (B + E)^T |_S - (B + E)(A + E)^{-1}(B + E)^T \right\| \quad (3.45)$$

$$+ \left\| (B + E)|_S (A + E)^{-1} (B + E)^T |_S - \left( (B + E)|_S (A + E)^{-1} (B + E)^T |_S \right) \Big|_S \right\| \quad (3.46)$$

$$\leq 32 (\mathcal{E} + \mathcal{E}^2) (\lambda_{\max} + \lambda_{\max}^2) \left( \left( \frac{2}{\lambda_{\min}^2} + 1 \right) \right) \quad (3.47)$$

$$+ \left\| (B)|_S (A)^{-1} (B)^T |_S - (B)(A)^{-1}(B)^T \right\| \quad (3.48)$$

$$+ \left\| B|_S (A)^{-1} B^T |_S - \left( B|_S (A)^{-1} B^T |_S \right) \Big|_S \right\| \quad (3.49)$$

$$\leq 32 (\mathcal{E} + \mathcal{E}^2) (\lambda_{\max} + \lambda_{\max}^2) \left( \left( \frac{2}{\lambda_{\min}^2} + 1 \right) \right) + 4\kappa^2 \lambda_{\max} N^2 C_\gamma \exp(-\gamma \rho_{\min}) \quad (3.50)$$

multiplying with a factor of  $N^2$  to obtain an estimate in Frobenius norm, we obtain the result.  $\square$

Next, we will turn this estimate for the error estimation in a single step into error estimate for all steps.

**Lemma 3.29.** Assume have for a sequence of positive real numbers,  $\mathcal{E}_0 = 0$  and  $F(\lambda_{\min}\lambda_{\max}, N, C_\gamma) \geq 1$

$$\mathcal{E}_{k+1} \leq F(\lambda_{\min}\lambda_{\max}, N, C_\gamma) ((\mathcal{E} + \mathcal{E}^2) + \epsilon_{\rho_{\min}} + \epsilon_\tau) \quad (3.51)$$

Then we have for all  $1 \leq k \leq q$ :

$$\mathcal{E}_k \leq k (2F(\lambda_{\min}\lambda_{\max}, N, C_\gamma))^k (\epsilon_{\rho_{\min}} + \epsilon_\tau), \quad (3.52)$$

if

$$(\epsilon_{\rho_{\min}} + \epsilon_\tau) \leq \frac{1}{q (2F(\lambda_{\min}\lambda_{\max}, N, C_\gamma))^q} \quad (3.53)$$

*Proof.* The above result can be proved by a simple induction argument  $\square$

Based on the above, we can now prove the accuracy of Algorithm 9

**Theorem 3.30.** Assume there exists an  $\alpha > 0$ , such that  $\lambda_{\min}^{-1}, \lambda_{\max}, e^q \leq N^\alpha$ . Let furthermore the index set  $J$  and the hierarchical pseudometric  $d(\cdot, \cdot)$  and the sparsity set  $S$  satisfy Condition 3.16 with constants  $C_d, d$  and Condition 3.17 with constant  $C_b$ . And let the sparsity set  $S$  fulfill  $S_{\rho_{\min}} \subset S \subset S_{\rho_{\max}}$ . Let furthermore  $\Gamma \in \mathbb{R}^{J \times J}$  satisfy Condition 3.7 with constant  $\kappa$  and Condition 3.6 with constants  $C_\gamma, \gamma$ . Then there exists a constant  $C(\alpha\kappa, C_\gamma, \gamma, C_b)$  such that for

$$\rho_{\min}\tau > C \log^2(N) \quad (3.54)$$

the Algorithm 9 completes without encountering a singular pivot and the resulting factorisation  $L_{\rho, \tau}$  has the property, that

$$\log \left( \frac{1}{\|L_{\rho, \tau} L_{\rho, \tau}^T\|} \right) \leq C \log^2(N) - \min(\rho_{\min}, \tau) \quad (3.55)$$

and has time complexity bounded from above by  $C\rho_{\max}^{3d}\tau^{d+1}\log^2(N)N$  and space complexity bounded from above by  $C\rho_{\max}^d N$ . In particular by choosing  $\rho_{\min}$  large enough, an  $\epsilon$ -approximation  $\Gamma$  is obtained in time complexity  $C(\log(1/\epsilon) + \log^2(N))^{4d+1}\log^2(N)$ .

*Proof.* From the Conditions 3.7 and 3.6 the exponential decay of the inverses and Schur complement appearing in Algorithm 9 can be deduced by Lemma 3.10. Here, Condition 3.16 is used to bound the constants  $c_{I,d}$  appearing in Lemma 3.10. Then, using Lemma 3.28 and 3.29, the norm of the difference  $\|\mathbb{S}^k(\Gamma) - \tilde{\mathbb{S}}^k(\Gamma)\|$  can be bounded for all  $1 \leq k \leq q$  by  $N^{\beta q}(\exp(-\tilde{\gamma}\rho_{\min}) + \exp(-\tilde{\gamma}\tau))$ , for some  $C, \alpha$ . From this, by a similiar argument as in the proof of Lemma 3.28, and possibly increasing  $\beta$ , a bound on  $L - L_{\rho, \tau}$  of the above form can be established. Finally from this bound, by increasing  $\beta$  again, a bound on  $\|L_{\rho, \tau} L_{\rho, \tau}^T - \Gamma\|$  of the same form can be established. The bounds on the computational complexity follows then from Theorem 3.25.  $\square$

**Theorem 3.31** (Error Estimate). Assume  $\Gamma$  fulfils Condition 3.6 for constants  $\gamma$  and  $C$  and Condition 3.7 for  $\kappa$ . Assume furthermore, that for all  $1 \leq k \leq q$ ,  $x > 0$ :  $c_{J(k), d}(x) \leq c(x)$  and let  $\tilde{d} : J \times J \rightarrow \mathbb{R}$  be a symmetric, positive function such that  $\tilde{d} \leq d$  For  $\rho > 0$  define  $\Gamma^{(q), \rho}$  by:

$$\Gamma_{i,j}^{(q), \rho} := \begin{cases} \Gamma_{i,j}^{(q), \rho}, & \tilde{d}(i, j) \leq \rho \\ 0, & \text{else} \end{cases}$$

Define  $L^\rho$  the lower triangular matrix obtained from  $\Gamma^{(q), \rho}$  by performing Cholesky factorisation ignoring all write operations to entries  $(i, j)$ , such that  $d(i, j) > \rho$ . Then we have:

$$\|\Gamma^{(q)} - L^\rho L^{\rho, T}\|_\infty \leq c(\tilde{\gamma}/2) C \frac{\sqrt{\|\Gamma^{(q), -1}\| \|\Gamma^{(q)}\|} (\|\Gamma^{(q)}\| + \|\Gamma^{(q), -1}\|)}{2(1-r)^2} \exp\left(-\frac{\tilde{\gamma}}{2}\rho\right),$$

for

$$\tilde{\gamma} := \frac{\log(r)}{(1 + \log(c(\gamma/2)) + \log(C_k)) - \log(r)} \frac{\gamma}{2}$$

and  $r := \frac{1-\kappa}{1+\kappa}$ .

*Proof.* The proof follows from the above theorem with  $S := \{\tilde{d}\} \leq \rho$ , together with the decay estimate in theorem 3.12. We note that according to Theorem 3.12, the elements of the exact Cholesky factor  $L$  fulfill:

$$|L_{i,j}| \leq c(\tilde{\gamma}/2) C \frac{\sqrt{\|\Gamma^{(q),-1}\|} (\|\Gamma^q\| + \|\Gamma^{(q),-1}\|)}{2(1-r)^2} \exp\left(-\frac{\tilde{\gamma}}{2}\rho\right),$$

for  $\tilde{d}(i,j) > \rho$ . Since furthermore  $L_{i,i} \leq \|\Theta\|$ , we have

$$L^\rho L^{\rho,T} = \Theta^{(q)} - E,$$

where

$$|E_{i,j}| \leq c(\tilde{\gamma}/2) C \frac{\sqrt{\|\Gamma^{(q),-1}\|} (\|\Gamma^q\| + \|\Gamma^{(q),-1}\|)}{2(1-r)^2} \exp\left(-\frac{\tilde{\gamma}}{2}\rho\right).$$

□

### 3.5 Validity of the conditions

In Owhadi and Scovel (2017), the authors give very general conditions under which the above conditions on exponential decay and bounded condition numbers are fulfilled. Following Owhadi and Scovel (2017), the abstract setting will consist of a Banach space  $\mathcal{B}$  and its topological dual  $\mathcal{B}^*$ , an continuous operator  $G : \mathcal{B}^* \rightarrow \mathcal{B}$  and its continuous inverse  $\mathcal{L}$ . For an arbitrary operator  $T : V \rightarrow W$ , we denote by  $C_T := \sup_{v \in V} \frac{\|Tv\|_W}{\|v\|_V}$  its continuity constant. We furthermore assume that we are given families of elements of  $\mathcal{B}^*$ ,  $\{\phi_i^{(k)}\}_{i \in I^{(k)}}$  for  $1 \leq k \leq q$  and that these are nested in the sense that there exist matrices  $\pi^{(k,l)} \in \mathbb{R}^{I^{(k)} \times I^{(l)}}$  for all  $1 \leq k \leq l \leq q$ , such that  $\phi_i^{(k)} = \sum_{j \in I^{(l)}} \pi_{i,j}^{(k,l)} \phi_j^{(l)}$ . Finally, we assume that we are given index sets  $J^{(k)}$  and matrices  $W^{(k)} \in \mathbb{R}^{J^{(k)} \times I^{(k)}}$ , for  $1 \leq k \leq q$ , such that  $\text{Im}(W^{(k),T}) = \text{Ker}(\pi^{(k-1,k)})$  and  $W^{(k)}W^{(k),T} = \text{Id}_{J^{(k)}}$ . For a Banach space  $V$  and its topological dual  $V^*$ , we denote by  $[\cdot, \cdot] : V \times V^* \rightarrow \mathbb{R}$  its duality product. In the following, we will deal with the following three examples. The first example is already treated in full, in (Owhadi and Scovel, 2017, Example 2.27), which is why we will mention it only briefly.

**Example 3.32** (Piecewise Polynomials). For  $s, d \in \mathbb{N}$ , let  $\Omega \subset \mathbb{R}^d$  be an open, bounded domain with Lipschitz boundary and  $\mathcal{B} = H_0^s(\Omega)$ . Let  $(h, \delta_{\text{mesh}}) \in (0, 1)$  and let  $\{\tau_t^{(k)}\}_{t \in T^{(k)}}$  be convex, uniformly Lipschitz domains that form a nested partition of  $\Omega$ , that is  $\Omega = \cup_{t \in T^{(k)}} \tau_t^{(k)}$  is a disjoint union except for the boundaries and each  $\tau_t^{(k)}$  can be written as the (up to boundaries) disjoint union of members of  $\{\tau_t^{(k)}\}_{t \in T^{(k+1)}}$ . Note, that we can choose  $\pi^{(k-1,k)}$  such that  $\|\pi^{(k-1,k)}\|_2 \leq C_\Phi$ . Assume, that  $\forall t \in T^{(k)}$ , there exists  $x_t^{(k)}$  such that

$$B_{\delta_{\text{mesh}} h^k}(x_t^{(k)}) \subset \tau_t^{(k)} \subset B_{h^k}(x_t^{(k)}) \quad (3.56)$$

Let for every  $t \in T^{(t)}$ ,  $\{\phi_{i,t}\}_{1 \leq i \leq \binom{s+d-1}{d}}$  be an  $L^2(\tau_t^{(k)})$  orthonormal basis of  $\mathcal{P}_{s-1}(\tau_t^{(k)})$ , the space of  $d$ -variate polynomials on  $\tau_t^{(k)}$  of degree at most  $s-1$ . Then define  $I^{(k)} := \{1, \dots, \binom{s+d-1}{d}\} \times T^{(k)}$  and let  $\phi_{i,t}^{(k)} := \phi_{i,t}$ , for  $(i, t) \in I^{(k)}$ . Choose  $W^{(k)}$ , such that  $\forall j \in J^{(k)}, \exists t \in T^{(k-1)}, \text{supp}(\phi_j^{(k),\chi}) \subset \tau_t^{(k-1)}$ . Now define  $\Omega_t^{(k)} := B_{2h^k}(x_t^{(k)}) \cap \Omega$ . For  $i^{(k)} = (s, t) \in I^{(k)}$  and  $j = (\sigma, \tau) \in I^{(l)}$ , we then define the pseudometric  $d$  as follows:

$$d(i^{(k)}, j^{(l)}) := \inf \left\{ n | p_1^{(r_1)} = t, p_2^{(r_2)} \in I^{(r_2)}, \dots, p_{n+1}^{(r_{n+1})} = \tau, \right. \quad (3.57)$$

$$\left. \min(k, l) \leq r_1 \dots r_{n+1}, \Omega_m^{(s_m)} \cap \Omega_{m+1}^{(s_{m+1})} \neq \emptyset \right\} \quad (3.58)$$

In statistical applications, most often the kernel function is continuous and evaluated at a set of measurement points. In this case, we can use subsampling as an averaging scheme, allowing for a near linear complexity algorithm without the use of quadrature formulae. For the following two example, we introduce an additional domain  $\Omega' \supset \Omega$ , which will be the physical domain of the partial differential operator, as opposed to  $\Omega$ .

**Example 3.33** (Radon measures with compact support). For  $s > d/2$ , let  $\Omega \subset \Omega' \subset \mathbb{R}^d$ , define  $\mathcal{B} := H_0^s(\Omega')$  and let  $\Omega$  be bounded with uniformly Lipschitz boundary. For  $h, \delta_{\text{mesh}} \in (0, 1)$  and  $q \in \mathbb{N}$  let  $\{x_i^{(1)}\}_{i \in I^1} \subset \dots \subset \{x_i^{(q)}\}_{i \in I^{(q)}} \subset \Omega$  for nested index sets  $I^{(1)} \subset \dots \subset I^{(q)}$  be a hierarchy of point sets, such that

1.  $\sup_{x \in \Omega} \min_{i \in I^{(k)}} \text{dist}(x, x_i^{(k)}) \leq h^k$
2.  $\inf_{i \neq j \in I^{(k)}} \text{dist}(x_i^{(k)}, \partial\Omega \cup x_j^{(k)}) \geq 2\delta_{\text{mesh}} h^k$ .

Let the constants  $\alpha_{\min}, \alpha_{\max}$  be such that  $0 < \alpha_{\min} \leq \alpha_{\max} < \infty$  and define  $\phi_i^{(k)} := \mu_i^{(k)}$  to be pairwise distinct Radon measures such that the mass of  $\mu_i^{(k)}$  restricted to  $B_{\delta_{\text{mesh}} h^q/2}(x_i^{(k)})$  is bounded from below by  $\alpha_{\min}$  and the mass of  $\mu_i^{(k)}$  is bounded from above by  $\alpha_{\max}$ . Let the sets of radon measures be nested,  $\{\mu_i^{(1)}\}_{i \in I^{(1)}} \subset \dots \subset \{\mu_i^{(q)}\}_{i \in I^{(q)}}$  and define

$$\pi_{i,j}^{(k,l)} := \begin{cases} 1, & \mu_i^{(k)} = \mu_j^{(l)} \\ 0, & \text{else} \end{cases} \quad (3.59)$$

Furthermore define  $J^k := I^{(k)} \setminus I^{(k-1)}$  (where  $I^{(0)} := \emptyset$ ) and

$$W_{i,j}^{(k)} := \delta_{i,j}. \quad (3.60)$$

The definition of  $\pi$  and  $W$  in are illustrated in Figure 7. Now define  $\Omega_i^{(k)} := B_{2h^k}(x_i^{(k)}) \cap \Omega$ . For  $i^{(k)} \in I^{(k)}$  and  $j \in I^{(l)}$ , we then define the pseudometric  $d$  as follows:

$$d(i^{(k)}, j^{(l)}) := \inf \left\{ n \mid p_1^{(r_1)} = i^{(k)}, p_2^{(r_2)} \in I^{(r_2)}, \dots, p_{n+1}^{(r_{n+1})} = j^{(l)}, \right. \quad (3.61)$$

$$\left. \min(k, l) \leq r_1 \dots r_{n+1}, \Omega_m^{(s_m)} \cap \Omega_{m+1}^{(s_{m+1})} \neq \emptyset \right\} \quad (3.62)$$

In some cases, the underlying PDE might not have enough regularity allow for pointwise evaluations of the Green's function. In this case, the question of whether subsampling can be used as an aggregation scheme becomes more difficult to answer. In order to treat this case, we present a third possible setting.

**Example 3.34** (Averaging over Patches). For  $s, d \in \mathbb{N}$ , let  $\Omega \subset \Omega' \subset \mathbb{R}^d$ , define  $\mathcal{B} := H_0^s(\Omega')$  and let  $\Omega$  be bounded with uniformly Lipschitz boundary. Let  $(h, \delta_{\text{mesh}}) \in (0, 1)$  and let  $\{\tau_i^{(k)}\}_{i \in I^{(k)}}$  be convex, uniformly Lipschitz domains that form a nested partition of  $\Omega$ , that is  $\Omega = \cup_{i \in I^{(k)}} \tau_i^{(k)}$  is a disjoint union except for the boundaries and each  $\tau_i^{(k)}$  can be written as the (up to boundaries) disjoint union of members of  $\{\tau_i^{(k)}\}_{i \in I^{(k+1)}}$ . Assume, that for all  $i \in I^{(k)}$ , there exists  $x_i^{(k)}$  such that

$$B_{\delta_{\text{mesh}} h^k}(x_i^{(k)}) \subset \tau_i^{(k)} \subset B_{h^k}(x_i^{(k)}). \quad (3.63)$$

Then define  $\phi_i^{(k)} := \frac{\mathbb{1}_{\tau_i^{(k)}}}{\sqrt{|\tau_i^{(k)}|}}$ ,

$$\pi_{i,j}^{(k,l)} := \begin{cases} \frac{\sqrt{|\tau_j^{(k+1)}|}}{\sqrt{|\tau_i^{(k)}|}}, & \tau_j^{(k+1)} \subset \tau_i^{(k)} \\ 0, & \text{else} \end{cases} \quad (3.64)$$

and define  $W^{(k)}$ , as described in (Owhadi, 2017, Construction 4.13), such that

1.  $\forall 1 \leq k < l \leq q, \forall i \in I^{(k)}, j \in J^{(k+1)}, \langle \phi_i^{(k)}, \phi_j^{(k+1), \chi} \rangle_{L^2} = 0.$
2.  $\forall 1 \leq k \leq q, \forall j \in J^{(k)}, \exists i \in I^{(k-1)} \text{ s.t. } \text{supp}(\phi_j^{(k), \chi}) \subset \tau_i^{(k-1)}.$
3.  $W^{(k)} W^{(k), T} = \text{Id}_{J^{(k)}}.$

Now define  $\Omega_t^{(k)} := \mathcal{B}_{2h^k}(x_t^{(k)}) \cap \Omega$ . For  $i^{(k)} \in I^{(k)}$  and  $j \in I^{(l)}$ , we then define the pseudometric  $d$  as follows:

$$d(i^{(k)}, j^{(l)}) := \inf \left\{ n | p_1^{(r_1)} = t, p_2^{(r_2)} \in I^{(r_2)}, \dots, p_{n+1}^{(r_{n+1})} = \tau, \right. \quad (3.65)$$

$$\left. \min(k, l) \leq r_1 \dots r_{n+1}, \Omega_m^{(s_m)} \cap \Omega_{m+1}^{(s_{m+1})} \neq \emptyset \right\} \quad (3.66)$$

We note that the last case was already treated in Owhadi (2017) and Owhadi and Scovel (2017, Example 2.26) for the case  $s = 1$ . In the following we extend the results there, by showing, that the polynomial order of the  $\phi_{i^{(k)}}$  need not match the order of the PDE.

### 3.5.1 Bounded condition numbers without vanishing moments

Hou and Zhang (2017) requires polynomial measurement functions  $\phi_i^{(k)}$  of order  $s - 1$  to prove the exponential decay of strongly elliptic differential operators of order  $2s$ . Although Owhadi and Scovel (2017) does not require polynomial measurement functions (or vanishing moments) to obtain the exponential decay of gambles for elliptic operators of order  $2s$ , a vanishing moments condition is implicitly used to obtain a uniform bound on the condition numbers of the matrices  $B^{(k)}$ . Vanishing moments conditions have also been used to compress integral operators with wavelets ( DeVore and Kunoth, 2009; Beylkin et al., 1991; Gines et al., 1998; Beylkin and Coult, 1998; Beylkin, 1998).

In the following, we will generalize the proof that the condition numbers of the matrices  $B^{(k)}$  are uniformly bounded (Owhadi and Scovel, 2017) by relaxing conditions requiring vanishing moments. As a result we will derive an *easy to implement* multi-resolution decomposition algorithm that does not require the prior construction of hierarchies of measurement functionals  $\phi_i^{(k)}$  with vanishing moments (with this generalization a simple sub-sampling strategy can be used to produce the  $\phi_i^{(k)}$ ).

The conditions, derived in Owhadi and Scovel (2017), for the uniform bound on the condition numbers of  $B^{(k)}$  are as follows:

**Condition 3.35.** There exists some constants  $C_\Phi \geq 1$  and  $H \in (0, 1)$  such that

1.  $\frac{1}{C_\Phi} H^k \leq \frac{\|\phi\|_*}{|x|}$  for  $k \in \{1, \dots, q\}$ ,  $x \in \mathbb{R}^{I^{(k)}}$  and  $\phi = \sum_{i \in I^{(k)}} x_i \phi_i^{(k)}$ . and  $x \in \mathbb{R}^{I^{(q)}}$ .
2.  $\frac{\|\phi\|_*}{|x|} \leq C_\Phi$  for  $\phi = \sum_{i \in I^{(1)}} x_i \phi_i^{(1)}$  and  $x \in \mathbb{R}^{I^{(1)}}$ .
3.  $\|\pi^{(k-1, k)}\|_2 \leq C_\Phi$  for  $k \in \{2, \dots, q\}$ .
4.  $\frac{1}{C_\Phi} J^{(k)} \leq W^{(k)} W^{(k), T} \leq C_\Phi J^{(k)}$  for  $k \in \{2, \dots, q\}$ .

and

**Condition 3.36.** The constants  $C_\Phi$  and  $H$  in Condition 3.35 satisfy also:

1.  $\inf_{\phi' \in \Phi^{(k-1)}} \frac{\|\phi - \phi'\|}{|x|} \leq C_\Phi H^{(k-1)}$  for  $\phi = \sum_{i \in I^{(k)}} x_i \phi_i^{(k)}$ ,  $k \in \{2, \dots, q\}$ , and  $x \in \mathbb{R}^{I^{(k)}}$ .
2.  $\frac{\|\phi\|_*}{|x|} \leq C_\Phi H^{(k-1)}$  for  $\phi = \sum_{i \in I^{(k)}} x_i \phi_i^{(k)}$ ,  $k \in \{2, \dots, q\}$ , and  $x \in \text{Ker}(\pi^{(k-1, j)})$ .

Conditions 3.35 play the role of an inverse Poincaré inequality, a global Poincaré inequality as well as bounds on the aggregation and orthogonalisation matrices. The first part of Condition 3.36 ensures that the operator is approximated better and better by its projection onto  $\Phi^{(k)}$  for growing  $k$ . We note that the second part of Condition 3.36 is a type of Poincaré inequality that actually implies the approximation property. The bounded condition numbers of  $B^{(k)}$  can be seen as arising from the balance between the inverse Poincaré inequality, which describes how higher eigenvalues of  $\mathcal{L}$  become visible under refinement of the mesh, and the Poincaré inequality, which describes how lower eigenvalues are factored out by the orthogonalisation procedure. The proof of the inverse Poincaré inequality depends only on localisation and scaling and will, for partial differential operators of order  $2s$ , generally yield  $H = h^{2s}$ . The Poincaré inequality however depends crucially on vanishing moments of order  $s - 1$ , in order to obtain the scaling  $H = h^{2s}$ , as was observed by Owhadi and Scovel (2017). This leads to the problem that the order of the operator as well as a suitable notion of polynomials have to be specified by the user and subsampling, the sparsest possible aggregation scheme, is ruled out. We will now prove that the following quantitative approximation property, which can be seen as an interpolation between the Poincaré inequality and the approximation property, is sufficient to obtain bounded condition numbers.

**Condition 3.37.** The constants  $C_\Phi$  and  $H$  in Condition 3.36 also satisfy

$$\inf_{y \in \mathbb{R}^{I^{(k-1)}}, |y| \leq C_\Phi |x|} \frac{\|\phi - \sum_{i \in I^{(k-1)}} y_i \phi_i^{(k-1)}\|_*}{|x|} \leq C_\Phi H^{k-1}$$

for  $\phi = \sum_{i \in I^{(k)}} x_i \phi_i^{(k)}$ ,  $k \in \{2, \dots, q\}$ , and  $x \in \mathbb{R}^{I^{(k)}}$ .

The following theorem is proved by a modification of (Owhadi and Scovel, 2017, Theorem 9.10).

**Theorem 3.38.** *Under Conditions 3.36 and 3.37 it holds true that there exists a constant  $C$  depending only on  $C_\Phi$  such that  $C^{-1}I^{(1)} \leq A^{(1)} \leq CH^{-2}I^{(1)}$ ,  $\text{Cond}(A^{(1)}) \leq CH^{-2}$ , and  $C^{-1}H^{-2(k-1)}J^{(k)} \leq B^{(k)} \leq CH^{-2k}J^{(k)}$  for  $k \in \{2, \dots, q\}$ . In particular,*

$$\text{Cond}(B^{(k)}) \leq CH^{-2}.$$

*Proof.* The proof of Theorem 3.38 is similar to that of (Owhadi and Scovel, 2017, Theorem 9.10) (and Theorem (Owhadi and Scovel, 2017, Theorem 10.9)). There are two important modifications. First observe that Condition 3.37 is sufficient to obtain (Owhadi and Scovel, 2017, Eq. 15.4)  $(z^T B^{(k)} z \leq C_\Phi^2 H^{-2(k-1)} |A^{(k)} W^{(k), T} z|^2)$  because the infimum in (Owhadi and Scovel, 2017, Eq. 15.3)  $(z^T B^{(k)} z = \inf_{y \in \mathbb{R}^{I^{(k-1)}}} \|\sum_{j \in J^{(k)}} z_j \chi_j^{(k)} - \sum_{i \in I^{(k-1)}} y_i \psi_i^{(k-1)}\|^2)$  is achieved for  $y = 0$ . Second, following Lemma (Owhadi and Scovel, 2017, Lemma 10.10), to bound  $\|P^{(k)}\|_2$  we modify lemmas (Owhadi and Scovel, 2017, Lemma 10.11) and (Owhadi and Scovel, 2017, Lemma 10.12) as follows. For  $x \in \mathbb{R}^{I^{(k)}}$  and  $y \in \mathbb{R}^{I^{(k-1)}}$ , we have  $P^{(k)}x = P^{(k)}(x - \pi^{(k,k-1)}y) + P^{(k)}\pi^{(k,k-1)}y$ . Using  $P^{(k)} = \pi^{(k,k-1)}A^{(k-1)}\pi^{(k-1,k)}\Theta^{(k)}$  we obtain that  $P^{(k)}\pi^{(k,k-1)}y = \pi^{(k,k-1)}y$  and  $|P^{(k)}(x - \pi^{(k,k-1)}y)| \leq \|\pi^{(k,k-1)}A^{(k-1)}\pi^{(k-1,k)}(\Theta^{(k)})^{\frac{1}{2}}\|_2 |x - \pi^{(k,k-1)}y|_{\Theta^{(k)}}$ . Choosing  $y$  as in Condition 3.37 and using  $\|\pi^{(k,k-1)}\|_2 \leq C_\Phi$  we deduce that  $|\pi^{(k,k-1)}y| \leq C_\Phi^2 |x|$  and  $|x - \pi^{(k,k-1)}y|_{\Theta^{(k)}} \leq C_\Phi H^{k-1} |x|$ . As in the proof of (Owhadi and Scovel, 2017, Lemma 10.11) observe that  $\|\pi^{(k,k-1)}A^{(k-1)}\pi^{(k-1,k)}(\Theta^{(k)})^{\frac{1}{2}}\|_2^2 = \lambda_{\max}(\pi^{(k,k-1)}A^{(k-1)}\pi^{(k-1,k)})$  and as in (Owhadi and Scovel, 2017, Eq. 10.34) bound  $\lambda_{\max}(\pi^{(k,k-1)}A^{(k-1)}\pi^{(k-1,k)})$  by  $\|\pi^{(k,k-1)}\|_2^2 \lambda_{\max}(A^{(k-1)}) \leq C_\Phi^4 H^{-2(k-1)}$ . Summarising we have obtained that

$$\|P^{(k)}\|_2 \leq C_\Phi^2 + C_\Phi^3.$$

The remaining part of the proof is similar to that of Theorem 10.9 of Owhadi and Scovel (2017).  $\square$

We first prove, that the quantitative approximation property and the inverse Poincaré inequality can be deduced from a simple scaling criterion:

**Theorem 3.39.** *Let  $\Omega \subset \Omega' \subset \mathbb{R}^d$  and let  $\Omega$  be bounded with uniformly Lipschitz boundary and let  $G$  be a continuous bijection from  $H^{-s}(\Omega')$  to  $H_0^s(\Omega')$  with inverse  $\mathcal{L}$ . For  $h, \delta_{\text{mesh}} \in (0, 1)$  and  $1 \leq k \leq q \in \mathbb{N}$  let  $\{x_i^{(k)}\}_{i \in I^k}$  sets of points in  $\mathbb{R}^d$ , such that*



1.  $\sup_{x \in \Omega} \min_{i \in I^{(k)}} \text{dist} \left( x, x_i^{(k)} \right) \leq h^k$
2.  $\inf_{i, j \in I^{(k)}} \text{dist} \left( x_i^{(k)}, \partial \Omega \cap x_j^{(k)} \right) \geq 2\delta_{\text{mesh}} h^k$

Let furthermore be  $0 < \alpha_{\min} \leq \alpha_{\max} < \infty$  and define  $\phi_i^{(k)} := \mu_i^{(k)}$  to be a Radon measure with mass bounded from below by  $\alpha_{\min}$  and from above by  $\alpha_{\max}$ , such that  $\text{supp} \left( \mu_i^{(k)} \right) \subset B_{h^k}(x_i^{(k)})$  and  $\phi_i^{(q)} \in (H_0^{-s}(\Omega'))$ .

Now define the functions

$$S_{\min}^{(k)}(r) := \min_{i \in I^{(k)}} \left\| \phi_i^{(k)} \right\|_{\left( H_0^s(B_r(x_i^{(k)})) \right)^*}$$

and

$$S_{\max}^{(k)}(r) := \max_{i \in I^{(k)}} \left\| \phi_i^q \right\|_{\left( H_0^s(B_r(x_i^{(k)})) \right)^*}$$

Then we have, for constants  $C_\Phi$  and  $r$  depending only on  $s, d, \Omega, \Omega', G, h, \delta_{\text{mesh}}, \alpha_{\max}/\alpha_{\min}$

1.  $\frac{1}{C_\Phi} S_{\min}^{(k)}(\delta_{\text{mesh}} h^k) \leq \frac{\|\phi\|_*}{|x|}$  for  $k \in \{1, \dots, q\}$ ,  $x \in \mathbb{R}^{I^{(k)}}$  and  $\phi = \sum_{i \in I^{(k)}} x_i \phi_i^{(k)}$ . and  $x \in \mathbb{R}^{I^{(q)}}$ .
2.  $\frac{\|\phi\|_*}{|x|} \leq C_\Phi S_{\max}^{(1)}(r)$  for  $\phi = \sum_{i \in I^{(1)}} x_i \phi_i^{(1)}$  and  $x \in \mathbb{R}^{I^{(1)}}$ .
3.  $\inf_{y \in \mathbb{R}^{I^{(k-1)}}, |y| \leq C_\Phi |x|} \frac{\|\phi - \sum_{i \in I^{(k-1)}} y_i \phi_i^{(k-1)}\|_*}{|x|} \leq C_\Phi S_{\max}^{(k)}(r h^{k-1})$ , for  $\phi = \sum_{i \in I^{(k)}} x_i \phi_i^{(k)}$ ,  $k \in \{2, \dots, q\}$ .

*Proof.* For part 2, we notice that by choosing  $r$  such that  $\Omega \subset B_{r-2/2}(0)$ , we obtain:

$$\sup_{v \in H_0^s(\Omega')} \frac{[\phi_i^q, v]}{\|v\|_{H_0^s(\Omega')}} \leq \sup_{v \in H^s(\Omega' \cap B_{(r/2-1)/2}(x_i^{(q)}))} \frac{[\phi_i^q, v]}{\|v\|_{H^s(\Omega' \cap B_{r/2-1}(x_i^{(q)}))}} \quad (3.67)$$

$$\leq C \sup_{v \in H_0^s(\Omega' \cap B_{r/2-1}(x_i^{(q)}) + B_1(0))} \frac{[\phi_i^q, v]}{\|v\|_{H_0^s(\Omega' \cap B_{r/2-1}(x_i^{(q)}) + B_1(0))}} \leq C \sup_{v \in H_0^s(B_{r/2}(x_i^{(q)}))} \frac{[\phi_i^q, v]}{\|v\|_{H_0^s(B_{r/2}(x_i^{(q)}))}} \quad (3.68)$$

$$\leq S_{\max}^{(1)}(r) \quad (3.69)$$

Here, the constant  $C$  follows from the application of a continuous extension theorem for Sobolev spaces, which can be obtained from the classical extension theorem to  $H_0^s(\mathbb{R})$  (Adams and Fournier, 2003) by application of a cutoff function. Now to prove part one, we can write, following Owhadi and Scovel (2017, Proposition 4.17):

$$\|\phi\|_{H^{-s}(\Omega')}^2 \geq \sum_{i \in I^{(k)}} \sup_{v_i \in H_0^s(B_{\delta_{\text{mesh}} h^k}(x_i))} \left[ 2 \int_{B_{\delta_{\text{mesh}} h^k}(x_i^{(k)})} x_i^{(k)} v_i \phi_i^{(k)} - \|v\|_{H_0^s(B_{\delta_{\text{mesh}} h^k}(x_i^{(k)}))}^2 \right] \quad (3.70)$$

$$= \sum_{i \in I^{(k)}} x_i^2 \left\| \phi_i^{(k)} \right\|_{H^{-s}(B_{\delta_{\text{mesh}} h^k}(x_i^{(k)}))}^2 \geq S_{\min}^{(k)}(\delta_{\text{mesh}} h^k/2)^2 |x|^2 \quad (3.71)$$

Next we prove part three. The proof will be similar to the proof of the first part of Condition 3.36, as found in the proof of (Owhadi and Scovel, 2017, Proposition 4.17).

By using a standard covering argument there exist  $h_0(\Omega)$ , and constants  $0 < c_{\min}(\Omega) \leq c_{\max}(\Omega)$  such that for every  $x_i^k$  with  $h^k \leq h_0$  there exists a matrix  $T \in \mathbb{R}^{d \times d}$  such that  $c_{\min} \leq \sigma_{\min}(T) \leq \sigma_{\max}(T) \leq c_{\max}$  such that

$$\Omega_i^{(k)} := T \left( \left[ 0, \frac{(2s+1)h^{k-1}}{\delta} \right]^d \right) + x_i^{(k)} \subset \Omega$$

where  $\delta = \delta(2s, d)$  is chosen according to Lemma 3.40. Therefore, by Lemma 3.40 there exists a  $0 < \rho_{\max}(\Omega, s)$  and  $C(\Omega, s)$  such that for all  $k$  with  $h^{k-1} \leq h_0$  and  $i \in I^{(k)}$  we have  $\text{diam}(\Omega_i^{(k)}) \leq \rho h^{k-1}$  and there exists  $w^{(i,k)} \in \mathbb{R}^{I^{(k-1)}}$  such that  $|w^{(i,k)}| \leq \alpha_{\max}/\alpha_{\min}C$  and

$$\int_{\Omega_i^{(k)}} p(x) \left( \phi_i^{(k)} - \sum_{j \in I^{(k-1)}} w_j^{(i,k)} \phi_j^{(k-1)} \right) = 0,$$

for all  $p \in \mathcal{P}_{2s-1}$ . We observe, that there exists a constant  $C_{\text{packing}}(d, \rho, \delta_{\text{mesh}})$ , such that

$$\# \{j | B_{\rho h^{k-1}}(x_i^{(k)}) \cap B_{\rho h^{k-1}}(x_j^{(k)}) \neq \emptyset\} \leq C_{\text{packing}}$$

Based on the above preparation, we want to prove the inequality for a given scale  $k$ . By estimating the remaining level by the Poincaré inequality on  $\Omega$ , we can restrict ourselves to the  $k$ , for which  $h^{k-1} \leq h_0$ . We set

$$y_i := x_i \sum_{j \in I^{(k-1)}} w_j^{(i,k)}$$

and compute:

$$\left\| \phi - \sum_{i \in I^{(k-1)}} y_i \phi_i^{(k-1)} \right\|_*^2 = \left\| \sum_{i \in I^{(k)}} x_i \phi_i^{(k)} - x_i \sum_{j \in I^{(k-1)}} w_j^{(i,k)} \phi_j^{(k-1)} \right\|_*^2 \quad (3.72)$$

$$= \sup_{v \in H_0^s(\Omega')} \left( 2 \sum_{i \in I^{(k)}} \left[ \int_{\Omega} v \left( x_i \phi_i^{(k)} - x_i \sum_{j \in I^{(k-1)}} w_j^{(i,k)} \phi_j^{(k-1)} \right) dx \right] - \|v\|_{H_0^s(\Omega')}^2 \right) \quad (3.73)$$

$$\leq \sup_{v \in H_0^s(\Omega')} \left( 2 \sum_{i \in I^{(k)}} \left[ \int_{\Omega} v \left( x_i \phi_i^{(k)} - x_i \sum_{j \in I^{(k-1)}} w_j^{(i,k)} \phi_j^{(k-1)} \right) dx \right] - \|v\|_{H_0^s(\Omega)}^2 \right) \quad (3.74)$$

$$\leq \sup_{v \in H_0^s(\Omega')} \left( 2 \sum_{i \in I^{(k)}} \left[ \int_{B_{\rho h^{k-1}}(x_i^{(k)})} v \left( x_i \phi_i^{(k)} - x_i \sum_{j \in I^{(k-1)}} w_j^{(i,k)} \phi_j^{(k-1)} \right) dx - \frac{1}{2C_{\text{packing}}} \|v\|_{H_0^s(B_{\rho h^{k-1}}(x_i^{(k)}))}^2 \right] \right) \quad (3.75)$$

$$= \sup_{v \in H_0^s(\Omega')} \left( 2 \sum_{i \in I^{(k)}} \inf_{p \in \mathcal{P}_{2s-1}(B_{\rho h^{k-1}}(x_i^{(k)}))} \left[ \int_{B_{\rho h^{k-1}}(x_i^{(k)})} (v - p) \left( x_i \phi_i^{(k)} - x_i \sum_{j \in I^{(k-1)}} w_j^{(i,k)} \phi_j^{(k-1)} \right) dx \right] \right) \quad (3.76)$$

$$- \frac{1}{2C_{\text{packing}}} \|v\|_{H_0^s(B_{\rho h^{k-1}}(x_i^{(k)}))}^2 \right] \quad (3.77)$$

Now, using the Bramble–Hilbert lemma (Bramble and Hilbert, 1970) in its version for convex domains, proven in Dekel and Leviatan (2004), we obtain from the above for a constant  $C(\Omega, \rho)$

$$\dots \leq \sup_{v \in H_0^s(\Omega')} \left( 2 \sum_{i \in I^{(k)}} \left[ Ch^{(k-1)s} \left\| x_i \phi_i^{(k)} - x_i \sum_{j \in I^{(k-1)}} w_j^{(i,k)} \phi_j^{(k-1)} \right\|_{(H^s(B_{\rho h^{k-1}}(x_i^{(k)})))^*} \|v\|_{H_0^s(B_{\rho h^{k-1}}(x_i^{(k)}))} \right] \right) \quad (3.78)$$

$$- \frac{1}{2C_{\text{packing}} h^d} \|v\|_{H_0^s(B_{\rho h^{k-1}}(x_i^{(k)}))}^2 \right] \quad (3.79)$$

$$\leq \left( \sum_{i \in I^{(k)}} \left[ Ch^{2(k-1)s} \left\| x_i \phi_i^{(k)} - x_i \sum_{j \in I^{(k-1)}} w_j^{(i,k)} \phi_j^{(k-1)} \right\|_{(H^s(B_{\rho h^{k-1}}(x_i^{(k)})))^*}^2 \right] \right), \quad (3.80)$$

where we used Young's inequality in the last step. Using the triangle inequality, we obtain:

$$\dots \leq Ch^{2(k-1)s} (|x|^2) \max \left( \left\{ \left\| \phi_i^{(k)} \right\|_{(H^s(B_{\rho h^{k-1}}(x_i^{(k)})))^*}^2 \mid i \in I^{(k)} \right\} \cup \left\{ \left\| \phi_i^{(k-1)} \right\|_{(H^s(B_{\rho h^{k-1}}(x_i^{(k)})))}^2 \mid i \in I^{(k)}, j \in I^{(k-1)} \right\} \right) \quad (3.81)$$

Now, we can compute:

$$\|\phi\|_{(H^s(B_{\rho h^{k-1}}(x_i^{(k)})))^*} = \sup_{v \in H^s(B_{\rho h^{k-1}}(x_i^{(k)}))} \frac{[\phi, v]}{\|v\|_{H^s(B_{\rho h^{k-1}}(x_i^{(k)}))}} \quad (3.82)$$

$$\leq h^{-d/2} \sup_{v \in H^s(B_{\rho h^{k-1}}(x_i^{(k)}))} \frac{[\phi, v]}{\|v(h^{k-1} \cdot)\|_{H^s(B_\rho(x_i^{(k)}))}} \quad (3.83)$$

$$\leq Ch^{-d/2} \sup_{v \in H^s(B_{\rho h^{k-1}}(x_i^{(k)}))} \frac{[\phi, v]}{\|E[v(h^{k-1} \cdot)]\|_{H_0^s(B_{2\rho}(x_i^{(k)}))}} \quad (3.84)$$

Here,  $E$  is the bounded extension operator from  $H^s(B_\rho(x_i^{(k)}))$  to  $H_0^s(B_{2\rho}(x_i^{(k)}))$ . By defining  $\tilde{v} := E[v(h^{k-1} \cdot)]$ , we obtain:

$$\|\phi\|_{(H^s(B_{\rho h^{k-1}}(x_i^{(k)})))^*} \leq Ch^{-d/2} \sup_{v \in H^s(B_{\rho h^{k-1}}(x_i^{(k)}))} \frac{[\phi, v]}{\|\tilde{v}\|_{H_0^s(B_{2\rho}(x_i^{(k)}))}} \quad (3.85)$$

$$\leq Ch^{-d/2} h^{-k-1} \sup_{v \in H^s(B_{\rho h^{k-1}}(x_i^{(k)}))} \frac{[\phi, v]}{\|\tilde{v}(h^{-(k-1)} \cdot)\|_{H_0^s(B_{2\rho}(x_i^{(k)}))}} \quad (3.86)$$

$$= Ch^{-d/2} h^{-k-1} \sup_{v \in H^s(B_{\rho h^{k-1}}(x_i^{(k)}))} \frac{[\phi, \tilde{v}(h^{-(k-1)} \cdot)]}{\|\tilde{v}(h^{-(k-1)} \cdot)\|_{H_0^s(B_{2\rho}(x_i^{(k)}))}} \quad (3.87)$$

$$\leq Ch^{-d/2} h^{-k-1} \|\phi\|_{(H^s(B_{2\rho h^{k-1}}(x_i^{(k)})))^*} \quad (3.88)$$

plugging this into our estimate of the dual norm, we obtain:

$$\left\| \phi - \sum_{i \in I^{(k-1)}} y_i \phi_i^{(k-1)} \right\|_*^2 \leq Ch^{-d/2} h^{-k-1} S_{\max}^{(k)} (r h^{k-1})$$

with  $r := 2\rho$ . □

**Lemma 3.40.** *Let  $m, d \in \mathbb{N}$ ,  $0 < \alpha_{\min} \leq \alpha_{\max} < \infty$  and  $r > 0$  be given. Then there exist constants  $\epsilon(m, d, \alpha_{\min}, \alpha_{\max}, r)$ ,  $\delta(m, d, r)$ , and  $n(m, d, \delta_{\text{mesh}})$  such that for all point sets  $\{x_i\}_{i \in I \cup \{0\}} \subset \mathbb{R}^d$  with  $\max_{x \in [0, \frac{(m+1)h}{\delta}]^d} \min_j \{\text{dist}(x, x_j)\} \leq h$  and all families of radon measure  $\{\mu_i\}_{i \in I \cup \{0\}}$  with mass between  $\alpha_{\min}$  and  $\alpha_{\max}$  and  $\text{supp}(\mu_i) \subset B_{rh}(x_i)$ , there exists a finite subset  $\{\nu_i\}_{i \in \{1 \dots n\}} \subset \{\mu_i\}_{i \in I}$  and  $w \in \mathbb{R}^n$  such that:*

$$[\mu_0, p] + \sum_{i=1}^n w_i [\nu_i, p] = 0, \quad \forall p \in \mathcal{P}_{m-1}([0, h/\delta]^d)$$

and  $|w|_2 \leq \epsilon^{-1}$ .

*Proof.* We first prove the result in the case, in which  $x_0 = 0$  and  $\mu_i := \delta_{x_i}$ . In this case, the problem has the following form:

$$p(0) + \sum_{i=1}^n w_i p(y_i) = 0, \quad \forall p \in \mathcal{P}_{m-1}([0, h/\delta]^d)$$

We remind ourselves that the problem of interpolating values at  $[1, \dots, m]^d$  with polynomials in  $\bigotimes_{k=1}^d \mathcal{P}_{m-1}(\mathbb{R})$  is uniquely solvable, in particular its Vandermonde matrix  $V(m, [1, \dots, m]^d)$  is invertible. By continuity of polynomials, there exists a  $0 < \delta(m, d) < 1/4$ ,  $0 < \epsilon(m, d)$  such that

$$\epsilon \leq \min \left\{ \sigma_{\min} \left( V(m, [1, \dots, m]^d + (z_1, \dots, z_m)) \right) \mid \sup_{1 \leq i \leq m} \{|z_i|\} < \delta \right\}.$$

That is, under perturbation of the grid smaller than  $\delta$ , the minimal singular value of  $V$  stays bounded below by  $\epsilon > 0$ . Notice, that the result of the lemma is invariant under rescaling of  $\{x_i\}_{i \in \mathbb{N}}$  and  $h$  by  $\frac{\delta}{h}$ , obtaining  $\tilde{h} := \frac{h}{\delta} h = \delta$  and  $\tilde{x}_i := \delta x_i$ . Then for each  $z \in [1, \dots, m]^d$  there exists an  $\tilde{x}_z \in \{\tilde{x}_i\}_{i \in I}$  such that  $|\tilde{x}_z - z| \leq \delta$ . We choose those elements our interpolation points and observe that we obtain the weights  $w_i$  as  $w := -V^{-1}(1, 0 \dots 0)$ . In particular we have correspondingly  $|w|_2 \leq \frac{1}{\epsilon}$ . This shows the result for Dirac measures. In order to extend the result to localised Radon probability measures, we initially proceed as in the above proof. In the very end, we can then decrease rescale with a factor depending only on  $r, s, d$  to “shrink the Radon measures to points”, until the generalised Vandermonde matrix is invertible. General but uniformly bounded masses can easily be incorporated by possibly including a factor of  $\alpha_{\max}/\alpha_{\min}$  in the norm estimate of  $w$ .  $\square$

**Remark 3.41.** We note, that the above described techniques to prove the bounds on the condition numbers are far more flexible than those based on vanishing moments. With our approach, the projection used in the proof and the projector used in the algorithm are decoupled, which allows us to use computationally nontrivial projectors in the proof, without needing to implement them in the algorithm.

If  $s > d/2$ , bounds on the  $S_{\max}$  and  $S_{\min}$  are particularly easy to establish:

**Theorem 3.42.** *In the setting of Example 3.33, we have, for a constant depending only on  $s, d, \Omega, \Omega', G, h, \delta_{\text{mesh}}, \alpha_{\max}/\alpha_{\min}$*

$$C^{-1} \alpha_{\max}^{-1} \prec A^{(1)} \prec \alpha_{\min}^{-1} h^{-2(s-d/2)}$$

and

$$C^{-1} \alpha_{\max}^{-1} h^{-2(k-1)(s-d/2)} \prec B^{(k)} \prec C \alpha_{\min}^{-1} h^{-2k(s-d/2)},$$

which results in

$$\begin{aligned} \text{cond} \left( A^{(1)} \right) &\leq C^2 \frac{\alpha_{\max}}{\alpha_{\min}} h^{-2(s-d/2)} \\ \text{cond} \left( B^{(k)} \right) &\leq C^2 \frac{\alpha_{\max}}{\alpha_{\min}} h^{-2(s-d/2)} \end{aligned}$$

*Proof.* Since obviously  $\|\pi^{(k-1, k)}\| = 1$  and  $W^{(k)} W^{(k), T} = \text{Id}$ , we need to show that the first two parts of Condition 3.35 and Condition 3.37 hold. We will use Theorem 3.39 and hence need to find bounds on  $S_{\min}$  and  $S_{\max}$ . The result follows directly from Theorem 3.39, provided we can bound  $S_{\min}$  from below and  $S_{\max}$  from above. Indeed, we have for some  $i, k$ :

$$\begin{aligned} S_{\max}^{(k)} \left( r h^{(k-1)} \right) &\leq \alpha_{\max} \sup_{v \in H_0^s(B_{r h^{k-1}}(x_i^{(k)}))} \frac{\|v\|_{C^0(B_{r h^{k-1}}(x_i^{(k)}))}}{\|v\|_{H_0^s(B_{r h^{k-1}}(x_i^{(k)}))}} \\ &\leq \alpha_{\max} r^{s-d/2} h^{(k-1)(s-d/2)} \sup_{v \in H_0^s(B_{r h^{k-1}}(x_i^{(k)}))} \frac{\|v(r h^{k-1} \cdot)\|_{C^0(B_1(x_i^{(k)}))}}{\|v(r h^{k-1} \cdot)\|_{H_0^s(B_1(x_i^{(k)}))}} \\ &\leq \alpha_{\max} C r^{s-d/2} h^{(k-1)(s-d/2)}, \end{aligned}$$

where the last estimate follows from the Sobolev embedding into Hölder spaces. In order to prove the lower bound on  $S_{\min}$ , let  $\eta \in H_0^s(B_1(0))$  be such that  $\eta \geq 0$  on  $\mathcal{B}_1(0)$  and  $\eta \geq 1$  on  $B_{1/2}(0)$ . We then have

$$\begin{aligned} \left\| \phi_i^{(k)} \right\|_{H^{-s}(B_{\delta_{\text{mesh}} h^k}(x_i^{(k)}))} &\geq \frac{\left[ \phi_i^{(k)}, \eta \left( x_i^{(k)} + 1/(\delta_{\text{mesh}} h^k)(\cdot) \right) \right]}{\left\| \eta \left( x_i^{(k)} + 1/(\delta_{\text{mesh}} h^k)(\cdot) \right) \right\|_{H_0^s(B_{\delta_{\text{mesh}} h^k}(x_i^{(k)}))}} \\ &\geq \frac{\alpha_{\min}}{\left\| \eta \left( x_i^{(k)} + 1/(\delta_{\text{mesh}} h^k)(\cdot) \right) \right\|_{H_0^s(B_{\delta_{\text{mesh}} h^k}(x_i^{(k)}))}} \\ &= \frac{(h^k \delta_{\text{mesh}})^{s-d/2} \alpha_{\min}}{\left\| \eta \right\|_{H_0^s(B_1(0))}}, \end{aligned}$$

from which follows  $S_{\min}^{(k)}(\delta_{\text{mesh}} h^k) \geq C \alpha_{\min} h^{k(s-d/2)}$ .  $\square$

Next we prove the bounded condition numbers in the case of averaging, by a similiar argument.

**Theorem 3.43.** *In the setting of Example 3.34, there exists a constant  $C$  depending only on  $s, d, \Omega, \Omega', C_G, C_{G^{-1}}, \delta_{\text{mesh}}$  such that*

$$C^{-1} h^{d/2} \prec A^{(1)} \prec \alpha_{\min}^{-1} h^{-2s}$$

and

$$C^{-1} h^{d/2} h^{-2(k-1)(s-d/2)} \prec B^{(k)} \prec C \alpha_{\min}^{-1} h^{-2ks},$$

which results in

$$\text{cond}(A^{(1)}) \leq C^2 h^{-d/2} h^{-2s}$$

$$\text{cond}(B^{(k)}) \leq C^2 h^{-d/2} h^{-2s}$$

*Proof.* By a simple calculation we see that  $\|\pi^{(k-1,k)}\| = 1$  and by construction  $W^{(k)} W^{(k),T} = \text{Id}$ . Again we need to show that the first two parts of Condition 3.35 Condition 3.37 hold. We want to use Theorem 3.39 but we first notice that the  $\phi_i^{(k)}$  are normalised in  $L^2$ , not in  $L^1$ , as is appropriate for the Radon measures used in Theorem 3.39. Therefore, we apply Theorem 3.39 to the rescaled  $\phi_i^{(k)}$ , normalised in the  $L^1$ -norm.

$$\begin{aligned} S_{\max}^{(k)}(r h^{(k-1)}) &\leq \frac{1}{\delta_{\text{mesh}}^d h^{kd}} \sup_{v \in H_0^s(B_{r h^{k-1}}(x_i^{(k)}))} \frac{\|v\|_{L^1(B_{r h^{k-1}}(x_i^{(k)}))}}{\|v\|_{H_0^s(B_{r h^{k-1}}(x_i^{(k)}))}} \\ &\leq \frac{1}{\delta_{\text{mesh}}^d h^{kd}} r^{s+d/2} h^{(k-1)(s+d/2)} \sup_{v \in H_0^s(B_{r h^{k-1}}(x_i^{(k)}))} \frac{\|v(r h^{k-1} \cdot)\|_{L^1(B_1(x_i^{(k)}))}}{\|v(r h^{k-1} \cdot)\|_{H_0^s(B_1(x_i^{(k)}))}} \\ &\leq \frac{r^{s+d/2}}{\delta_{\text{mesh}}^d} C h^{(k-1)(s+d/2)-kd}, \end{aligned}$$

where the last estimate follows from the Sobolev embedding into Hölder spaces. In order to prove the lower bound on  $S_{\min}$ , let  $\eta \in H_0^s(B_1(0))$  be such that  $\eta \geq 0$  on  $\mathcal{B}_1(0)$  and  $\eta \geq 1$  on  $B_{1/2}(0)$ . We then have

$$\frac{\left\| \phi_i^{(k)} \right\|_{H^{-s}(B_{\delta_{\text{mesh}} h^k}(x_i^{(k)}))}}{\sqrt{h^{kd} \pi}} \geq \frac{\left[ \phi_i^{(k)}, \eta \left( x_i^{(k)} + 1/(\delta_{\text{mesh}} h^k)(\cdot) \right) \right]}{\sqrt{\pi h^{kd}} \left\| \eta \left( x_i^{(k)} + 1/(\delta_{\text{mesh}} h^k)(\cdot) \right) \right\|_{H_0^s(B_{\delta_{\text{mesh}} h^k}(x_i^{(k)}))}}$$

$$\begin{aligned}
&\geq \frac{\delta_{\text{mesh}}^2}{2 \left\| \eta \left( x_i^{(k)} + 1 / (\delta_{\text{mesh}} h^k) (\cdot) \right) \right\|_{H_0^s(B_{\delta_{\text{mesh}} h^k}(x_i^{(k)}))}} \\
&= \frac{(h^k \delta_{\text{mesh}})^{s-d/2} \alpha_{\min}}{\|\eta\|_{H_0^s(B_1(0))}},
\end{aligned}$$

from which follows  $S_{\min}^{(k)}(\delta_{\text{mesh}} h^k) \geq C h^{k(s-d/2)}$ . By applying Theorem 3.39 and scaling back to normalisation with respect to  $L^2$ , we obtain

1.  $\frac{1}{C_\Phi} h^{ks} \leq \frac{\|\phi\|_*}{|x|}$  for  $k \in \{1, \dots, q\}$ ,  $x \in \mathbb{R}^{I^{(k)}}$  and  $\phi = \sum_{i \in I^{(k)}} x_i \phi_i^{(k)}$ . and  $x \in \mathbb{R}^{I^{(q)}}$ .
2.  $\frac{\|\phi\|_*}{|x|} \leq C_\Phi h^{-d/2}$  for  $\phi = \sum_{i \in I^{(1)}} x_i \phi_i^{(1)}$  and  $x \in \mathbb{R}^{I^{(1)}}$ .
3.  $\inf_{y \in \mathbb{R}^{I^{(k-1)}}, |y| \leq C_\Phi |x|} \frac{\|\phi - \sum_{i \in I^{(k-1)}} y_i \phi_i^{(k-1)}\|_*}{|x|} \leq C_\Phi h^{(k-1)s-d/2}$ , for  $\phi = \sum_{i \in I^{(k)}} x_i \phi_i^{(k)}$ ,  $k \in \{2, \dots, q\}$ .

The result follows then, by applying Theorem 3.38.  $\square$

Finally, for Example 3.32, from (Owhadi and Scovel, 2017, Proposition 2.17) and (Owhadi and Scovel, 2017, Theorem 2.13) follows:

**Theorem 3.44.** *In the setting of Example 3.32, we have, for a constant depending only on  $s, d, \Omega, G, \delta_{\text{mesh}}$*

$$C^{-1} \prec A^{(1)} \prec h^{-2s}$$

and

$$C^{-1} h^{-2(k-1)s} \prec B^{(k)} \prec C h^{-2ks},$$

which results in

$$\begin{aligned}
\text{cond}(A^{(1)}) &\leq C^2 h^{-2s} \\
\text{cond}(B^{(k)}) &\leq C^2 h^{-2s}
\end{aligned}$$

### 3.5.2 Exponential decay of gamblets

In this section, we will present the recent abstract results of exponential localisation of gamblets obtained in Owhadi and Scovel (2017), which in turn are a generalisation of the subspace iteration method introduced in Kornhuber and Yserentant (2016a,b). We note that, by generalising the arguments in Owhadi (2017) to higher order equations, exponential decay for higher order elliptic PDE was obtained by Hou and Zhang (2017) under the additional condition of strong ellipticity, independently of Owhadi and Scovel (2017).

The first ingredient for the proof exponential decay in Owhadi and Scovel (2017) will be a domain decomposition

**Construction 3.45.** Let  $\{\mathcal{B}_i^{(k)}\}_{i \in I^{(k)}}$  be a family of subspaces of  $\mathcal{B}$ , such that  $\mathcal{B} := \sum_{i \in I^{(k)}} \mathcal{B}_i^{(k)}$  and for all  $i \in I^{(k)}$ , there exists  $v_i^{(k)} \in \mathcal{B}_i^{(k)}$  such that  $[\phi_i^{(k)}, v_j^{(k)}] = \delta_{i,j}$ .

We define  $\mathfrak{V}^{(k), \perp} := \{v \in \mathcal{B} | [\phi_i^{(k)}, v] = 0, \forall i \in I^{(k)}\}$  and  $\mathfrak{V}_i^{(k), \perp} := \mathcal{B}_i \cap \mathfrak{V}^{(k), \perp}$ . We define  $P_i^{(k)}$  as the  $\langle \cdot, \cdot \rangle$ -orthogonal projection of  $\mathcal{B}$  onto  $\mathfrak{V}_i^{(k), \perp}$  and define  $P^{(k)} := \sum_{i \in I^{(k)}} P_i^{(k)}$ .

As before, we define the gamblets  $\psi_i^{(k)} := \mathbb{E}[u | [\phi_j^{(k)} = \delta_{i,j}]]$ , for  $u$  a centered gaussian vector with covariance operator  $G$ . Define the undirected graph  $G^{(k)} := (I^{(k)}, E^{(k)})$  such that  $\{i, j\} \in E$  iff there exist  $v_i \in \mathcal{B}_i^{(k)}$  and  $v_j \in \mathcal{B}_j^{(k)}$  such that  $\langle v_i, v_j \rangle \neq 0$ . Let  $d^{(k)}(\cdot, \cdot)$  denote the corresponding graph distance. Define  $\psi_i^{(k), 0}$  as the solution to:

$$\begin{cases} \text{Minimize } \|\psi\| \\ \text{Subject to } \psi \in \mathcal{B}_i^{(k)} \text{ and } [\phi_j^{(k)}, \psi] = \delta_{i,j} \end{cases}$$

Then Owhadi and Scovel (2017, Theorem 6.4.) states:

**Theorem 3.46.** *If  $\lambda_{\min}(P) > 0$ , then for all  $n > 0$  there exists a  $\psi_i^{(k),n} \in \sum_{j:d^{(k)}(i,j) \leq n} \mathcal{B}_j$ , such that*

$$\|\psi_i^{(k)} - \psi_i^{(k),n}\| \leq \left( \frac{\text{cond}(P) - 1}{\text{cond}(P) + 1} \right)^n \|\psi_i^{(k),0}\|$$

Owhadi and Scovel (2017) give methods for the estimation of  $\text{cond}(P)$ , which result in proofs of exponential decay. In the case where  $\mathcal{B}$  is a Sobolev space, the following construction is used.

**Construction 3.47** (Construction 2.19 in Owhadi and Scovel (2017)). Let  $h, \delta_{\text{mesh}} \in (0, 1)$ , for  $1 \leq k \leq q$  let  $\tau_i^{(k)}$  be a partition of the Lipschitz domain  $\Omega \subset \mathbb{R}^d$  into convex, uniformly Lipschitz sets such that contain a ball of radius  $\delta_{\text{mesh}} h^k$  and are contained in a ball of radius  $h^k$ , with  $\text{supp}(\phi_i^{(k)}) \subset \tau_i^{(k)}$ . For  $i \in I^{(k)}$ , let  $\Omega_i^{(k)} \subset \Omega$  such that  $\Omega_i^{(k)}$  contains  $\tau_i$  and  $\text{dist}(\Omega_i^{(k),c} \cap \Omega, \tau_i^{(k)}) \geq h^k$ . Then we can define  $\mathcal{B}_i^{(k)} := H_0^s(\Omega_i^{(k)})$ .

In order to prove exponential decay, the following condition is needed.

**Condition 3.48** (Condition 2.23 in Owhadi and Scovel (2017)). Given Construction 3.47 with  $\delta_{\text{mesh}}, h \in (0, 1)$ . And define

$$\mathfrak{V}^{(k),\perp} := \left\{ f \in H_0^s(\Omega) \mid [\phi_i^{(k)}, f] = 0, \forall i \in I^{(k)} \right\}.$$

Then we assume that there exists a constant  $C(\Omega, d, \delta_{\text{mesh}}, s, \Omega, s)$ , such that

$$\|D^t f\|_{L^2(\Omega)} \leq C h^{s-t} \|f\|_{H_0^s(\Omega)} \text{ for } t \in \{0, 1, \dots, s\}, f \in \mathfrak{V}^{(k),\perp}, \quad (3.89)$$

$$\sum_{i \in I^{(k)}} [\phi_i^{(k)}, f]^2 \leq C \left( \|f\|_{L^2(\Omega)}^2 + h^{2s} \|f\|_{H_0^s(\Omega)}^2 \right), f \in H_0^s(\Omega), \quad (3.90)$$

$$|x|^2 \leq C h^{-2s} \|\phi_i^{(k)}\|_{H^{-s}(\tau_i^{(k)})}, \forall i \in I^{(k)} \quad (3.91)$$

Under these conditions (Owhadi and Scovel, 2017, Theorem 6.20) proves exponential decay of Gamblots:

**Theorem 3.49.** *Given a bounded measurable open subset of  $\Omega \subset \mathbb{R}^d$  with uniformly Lipschitz boundary, let  $s \in \mathbb{N}^*$  and let  $\mathcal{L}$  be a continuous bijection from  $H_0^s(\Omega)$  to  $H^{-s}(\Omega)$  that is local in the sense that  $[\mathcal{L}v, v] = 0$  if  $\text{supp}(v) \cap \text{supp}(v') = \emptyset$ . Let  $C_{\mathcal{L}}, C_{\mathcal{L}^{-1}}$  be the continuity constants of  $\mathcal{L}$ . Let  $\phi_i^{(k)}$  be as in Construction 3.47 and satisfy Condition 3.48. Then there exists a constant  $C$  depending only on  $d, \delta_{\text{mesh}}, s, C_{\mathcal{L}}$  and  $C_{\mathcal{L}^{-1}}$  such that  $\text{cond}(P) \leq C$  and  $\|\psi_i^{(k),0}\| \leq C$ .*

Using the above cited theorems, we are now ready to prove the hierarchical exponential decay.

**Theorem 3.50.** *For  $s > d/2$ , and  $h, \delta_{\text{mesh}} \in (0, 1)$  consider the situation of Example 3.33, with  $\Omega = \Omega'$ . Let  $C_{\mathcal{L}}, C_{\mathcal{L}^{-1}}$  be the continuity constants of  $\mathcal{L}$  and its inverse. Then we have, for constant  $C, \gamma$  depending only on  $s, d, \Omega, \Omega', \delta_{\text{mesh}}, C_{\mathcal{L}}, C_{\mathcal{L}^{-1}}, \alpha_{\max}/\alpha_{\min}$ , that Condition 3.6 holds.*

*Proof.* When looking into the proof of Theorem 3.49 in Owhadi and Scovel (2017) one notices that the fact that the  $\Omega_i^{(k)}$  is derived from a partition  $\tau_i^{(k)}$  is not essential and the proof holds equally for  $\Omega_i^{(k)}$  as introduced above. We notice, that the exponential decay of gamblots as in the statement of Theorem 3.46 is invariant under scaling of  $\phi_i^{(k)}$ . Hence, to better fit to the notation in Owhadi and Scovel (2017, Proposition 13.3), we can instead treat the case of  $\tilde{\phi}_i^{(k)} := h^{kd/2} \phi_i^{(k)}$ . After this rescaling, the proof of the second and third estimate in Condition 3.48 is analogous to the case of Dirac measures treated in Owhadi and Scovel (2017, Proposition 13.3). In order to show that Condition 3.48 holds, we note that for  $f$  to integrate to zero against a Radon measure with support localised in  $B_\rho(x_i^{(k)})$  it has to have positive and negative values in  $B_\rho(x_i^{(k)})$ . Therefore, by the intermediate value theorem, it has to achieve the value 0 somewhere in  $B_\rho(x_i^{(k)})$ . Thus, the proof of the Poincaré inequality can be reduced to the one found in Owhadi and Scovel (2017, Proposition 13.3) for Dirac measures.

Therefore, one obtains the estimate

$$\left\| \psi_i^{(k)} - \psi_i^{(k),n} \right\| \leq C \exp^{-\gamma n}$$

Therefore we have

$$\left| \left( \left( \Gamma_{[k+1:q], [1:k]}^q \Gamma^{(k), -1} \right)_{l,1} \right)_{i,j} \right| = \left[ \phi_i^{(l)}, \psi_j^{(k)} \right] \leq C \exp(-\gamma d(i, j))$$

and

$$\left| \left( \Gamma_{i,j}^{(k), -1} \right) \right| = \left\langle \psi_i^{(k)}, \psi_j^{(k)} \right\rangle \leq C \exp(-\gamma d(i, j))$$

□

**Theorem 3.51.** For  $h, \delta_{\text{mesh}} \in (0, 1)$  consider the situation of Example 3.32, with  $\Omega = \Omega'$  and let  $\mathcal{L}$  be a continuous bijection from  $H_0^s(\Omega)$  to  $H^{-s}(\Omega)$  that is local in the sense that  $[\mathcal{L}v, v] = 0$  if  $\text{supp}(v) \cap \text{supp}(v') = \emptyset$ . Let  $C_{\mathcal{L}}, C_{\mathcal{L}^{-1}}$  be the continuity constants of  $\mathcal{L}$  and its invers. Then we have, for constants  $C, \gamma$  depending only on  $s, d, \Omega, \Omega', \delta_{\text{mesh}}, C_{\mathcal{L}}, C_{\mathcal{L}^{-1}}$ , that Condition 3.6 holds.

*Proof.* The result follows directly from Owhadi and Scovel (2017, Theorem 2.24) and Owhadi and Scovel (2017, Theorem 2.24) and the argument in Theorem 3.50. □

**Theorem 3.52.** For  $h, \delta_{\text{mesh}} \in (0, 1)$  consider the situation of Example 3.34, with  $\Omega = \Omega'$  and let  $\mathcal{L}$  be a continuous bijection from  $H_0^s(\Omega)$  to  $H^{-s}(\Omega)$  that is local in the sense that  $[\mathcal{L}v, v] = 0$  if  $\text{supp}(v) \cap \text{supp}(v') = \emptyset$ . Let  $C_{\mathcal{L}}, C_{\mathcal{L}^{-1}}$  be the continuity constants of  $\mathcal{L}$  and its invers. Then we have, for constants  $C, \gamma$  depending only on  $s, d, \Omega, \Omega', \delta_{\text{mesh}}, C_{\mathcal{L}}, C_{\mathcal{L}^{-1}}$ , that Condition 3.6 holds.

*Proof.* The result follows directly from Owhadi and Scovel (2017, Theorem 2.24) and Owhadi and Scovel (2017, Theorem 2.24) and the argument in Theorem 3.50. □

### 3.6 The final result

The combined results of the last subsection will now lead to proof of the correctness and runtime estimate of our algorithm.

**Theorem 3.53.** Consider the situation of Examples 3.33 3.32 or 3.34 with  $\Omega = \Omega'$ . Then, there exist constants  $C, c, \gamma, p$  depending only on  $s, d, \Omega, \delta_{\text{mesh}}, \alpha_{\min}, \alpha_{\max}, C_{\mathcal{L}}, C_{\mathcal{L}^{-1}}, h$  such that for a sparsity set  $S$  such that  $S_{\rho_{\min}} \subset S \subset S_{\rho_{\max}}$  and  $\rho_{\min}, \tau \geq Cq^2 \log^2 h$ , Algorithm 9 applied to  $\Gamma$  restricted to indices  $i, j$  with  $d(i, j) \leq \rho$  has the following approximation property:

$$\left\| \Gamma^{(q)} - L_{\rho, \tau} L_{\rho, \tau}^T \right\| \leq Ch^{-pq^2} (\exp(-\gamma\rho) + \exp(-\gamma\tau))$$

and has at most  $CN \log^2(N) \rho_{\max}^{3d} \tau^{d+1}$  time complexity and  $CN \log(N) \rho_{\max}^d$  space complexity.

Put another way, defining  $N := \#I^{(q)}$ , to achieve an  $\epsilon$ -approximation of  $\Gamma^q$ , one has time complexity  $\mathcal{O}\left(N \log^2(N) (\log(1/\epsilon) + \log^2(N))^{4d+1}\right)$  and space complexity  $\mathcal{O}\left(N \log(N) \left(\log^d\left(\frac{1}{\epsilon}\right) + \log^d(N)\right)\right)$ . In particular, only  $\mathcal{O}\left(N \log(N) (\log(\frac{1}{\epsilon}) + \log(N))\right)$  entries of  $\Gamma$  have even to be known to the user.

*Proof.* The result follows directly by putting together the results of the last section. From Theorems 3.50, 3.51, and 3.52, it follows that the Condition 3.6 on hierarchical exponential decay is satisfied. Similarly, from Theorems 3.42, 3.44, and 3.43 it follows, that Condition 3.7 on bounded condition numbers is satisfied. This results by theorem 3.31 in the approximation property as described above. Here we used Theorems 3.42, 3.44, and 3.43 to obtain the polynomial bounds on the norms of  $\Gamma$  and  $\Gamma^{-1}$ . It follows from a simple sphere packing argument that  $d$  fulfils the Conditions 3.16a and 3.17. The complexity estimate then follows from theorem 3.18. □

**Corollary 3.54.** In the above theorem,  $d(\cdot, \cdot)$  can be replaced with

$$\tilde{d}(i, j) := h^{-\min(k, l)} \text{dist}(x_i^{(k)}, x_j^{(l)}), \forall i \in J^{(k)}, j \in J^{(l)},$$

for a possibly different constant.

*Proof.* The corollary follows directly from the above theorem, since  $\tilde{d}(i, j) \leq Cd(i, j)$ , for a constant  $C$ , depending only on  $s, d, \Omega, \Omega', \delta_{\text{mesh}}, \alpha_{\min}, \alpha_{\max}, C_{\mathcal{L}}, C_{\mathcal{L}^{-1}}$ . □



### 3.7 Additional consequences of the result

#### 3.7.1 Sparse Cholesky decomposition of the stiffness matrix

In numerical analysis, instead of being given the matrix  $\Theta$ , many times one starts out with the inverse  $A$ , in the form of a discretised differential operator. In this case, the compression of the operator is not the main concern, since it will usually be banded according to the physical distance of the meshpoints. However, even though the original matrix might be sparse, its Cholesky factors won't be sparse because of the fill-in phenomenon. While there exist numerous approaches to finding orderings that reduce fill in, we are not aware of any such ordering that results in a provably near-linear algorithm on meshes in dimension  $d > 1$ . Often, the analysis of fill-in is based on graph theoretic approaches which, as in nested dissection ordering (George, 1973; Lipton et al., 1979; Gilbert and Tarjan, 1987) or minimal degree ordering (George and Liu, 1989). These methods however only exploit the algebraic structure implied by the position of the nonzero entries, without taking the values of these nonzero entries into consideration, a property that is very rigid with respect to small perturbations of the precision matrix. Instead, when interpreting the dense inverse matrix as a covariance operator corresponding to a smooth function prior it is very natural that the sparsity inducing effect of elimination should enjoy a certain robustness. This allows to replace the separators used in nested dissection by smaller “approximate” separators, leading to near-linear algorithms. Thus, probabilistic interpretation of the *fade-out* occurring during the decomposition of the inverse operator  $\Theta$  also gives a more complete understanding of the *fill-in* effect encountered when decomposing  $A$ . We have the following theorem:

**Theorem 3.55.** *Assume that  $\Theta$  has a Cholesky decomposition  $\Theta = LL^T$ , with:*

$$|L_{i,j}| \leq C \exp(-\gamma_L d(i, j))$$

*And that the inverse  $A := (\Theta)^{-1}$  decays as*

$$|A_{i,j}| \leq C \exp(-\gamma_A d(i, j)).$$

*Furthermore assume, that  $d(\cdot, \cdot)$  fulfils Conditions 3.16 and 3.17. Now define  $P$  as the permutation matrix reversing the order of variables. Then the Cholesky decomposition of  $PAP$  is exponentially localised as:*

$$|\tilde{L}_{i,j}| \leq qC^2 \tilde{C}(\gamma_A, \gamma_L) \exp(-(\gamma_A \gamma_L) / 4d(P[i], P[j]))$$

*where by a slight abuse of notation,  $P[i]$  is defined as the  $j$ , such that  $Pe_i = e_j$  and  $q$  denotes the number of levels of  $d$ . Furthermore, the Cholesky of  $PAP$  restricted to  $\{i, j | d(Pi, Pj) \leq \rho\}$  can be computed in the same time- and space complexity as the one of  $\Theta$  restricted to  $\{i, j | d(i, j) \leq \rho\}$ .*

*Proof.* We have:

$$A = (LL^T)^{-1} = L^{-T}L^{-1} \implies PAP = (PL^{-1}P)^{-T} PL^{-1}P.$$

We notice, that  $PL^{-1}P$  is an upper triangular matrix. Therefore, we know that the Cholesky factors of  $PAP$  are given by  $(PL^{-1}P)^{-T}$ . To show the required localisation, we have to show the localisation of  $L^{-1}$ . We have however

$$L(L^T A) = \text{Id} \implies L^{-1} = L^T A$$

Now, we note that when using the usual block structure induced by the multiresolution basis, the blocks  $(L^T)_{k,l}$  for  $l < k$  are zero. Hence, by the triangle inequality of  $d(\cdot, \cdot)$ ,  $L^{-1}$  is decaying exponentially as described above. As before, this shows the exponential accuracy of the restricted Cholesky factorisation. The space- and time complexity follows then from Lemma 3.14 by noticing, that under the reverse ordering  $S_\uparrow(i)$  and  $S_\downarrow(i)$  are interchanged.  $\square$

We note, that in a scenario where we are given the stiffness matrix, we will typically know the order of our operator. Furthermore, since the stiffness matrix is sparse, the application of averaging based multiresolution with vanishing moments will be possible in near linear time. Therefore, while subsampling based sparse Cholesky decomposition as in Theorem 3.53 is an option, we can also use a multiresolution basis as in Owhadi and Scovel (2017)[Example 2.27]. The results in this reference, which also motivated the present work, directly yield the Conditions 3.7 and 3.6.

### 3.7.2 The rank revealing property of sparsifying Cholesky decomposition

As was already noticed in Owhadi (2017), the upper and lower bounds on the condition number of the  $B^{(k)}$  together with the orthogonality in the operator inner product suggest that the gamblets have some similarity to an eigenspace decomposition, with the difference that they can be computed in near-linear time. While they are not orthogonal in  $L^2$ , as one would expect from an eigen-decomposition, it was shown in Owhadi and Scovel (2017) that the minimum angle between gamblets on different scales is bounded uniformly from below, which can be seen as a sort of “approximate orthogonality”. Hou and Zhang (2017) generalised the construction of Owhadi (2017) to higher order elliptic operators (independently of Owhadi and Scovel (2017)) and proposed its use for the compression of Green’s operators. Since the sparsifying Cholesky decomposition is intimately related to the gamblet transform, it inherits the PCA-like behaviour of the gamblets. Consider the following low-rank variant of the Cholesky decomposition where  $i^{(l)}$  denotes the largest index  $i$ , such that  $i \in I^{(l)}j$ .

---

**Algorithm 10:** Low rank Cholesky decomposition

---

**input** : A positive definite  $N \times N$  matrix  $\Theta$  and a maximum level  $k$   
**output**: A lower triangular  $N \times N$  matrix  $L$ .

**for**  $i \leftarrow 1$  **to**  $i^{(l)}$  **do**  
    **for**  $j \leftarrow i$  **to**  $N$  **do**  
         $L_{i,j} \leftarrow \Theta_{i,j}$

**for**  $i \leftarrow 1$  **to**  $i^{(l)}$  **do**  
    **for**  $j \leftarrow i + 1$  **to**  $i^{(l)}$  **do**  
         $L_{[j:N],j} \leftarrow L_{[j:N],j} - L_{[j:N],i}L_{j,i}/L_{i,i}$   
         $L_{i:N,i} \leftarrow L_{[i:N],i}/\sqrt{L_{i,i}}$

---

We have the following estimates for the truncation error of the low-rank Cholesky decomposition.

**Theorem 3.56.** *Assume the following conditions are fulfilled:*

1.  $\|\pi^{(l+1,q)}\|_2 \leq C$  for  $k \in \{2, \dots, q\}$ .
2.  $\frac{1}{C}J^{(l+1)} \leq W^{(l+1)}W^{(l+1),T} \leq CJ^{(l+1)}$ .
3.  $\inf_{\phi' \in \Phi^{(l)}} \frac{\|\phi - \phi'\|}{|x|} \leq CH^l$  for  $\phi = \sum_{i \in I^{(q)}} x_i \phi_i^{(q)}, x \in \mathbb{R}^{I^{(q)}}$ .

Then, for  $L^{(l)}$  being the output of the above algorithm applied to  $\Gamma$ , we have the following approximation result in the operator norm:

$$\left\| L^{(l)} L^{(l),T} - \Gamma \right\| \leq CH^{2l} J^{(l+1),-1}$$

*Proof.* We recognise that Algorithm 10 is equivalent to the assuming that after the outer iterations for  $i$  up to  $i^{(l)}$ , the remaining block on the lower right is zero. This can equally be achieved by subtracting this lower right block from  $\Theta$ , to begin with. It turns out that this lower right block is the Schur complement  $\Theta_{[l+1:q],[l+1:q]} - \Theta_{[l+1:q],[1:l]} (\Theta_{[1:l],[1:l]})^{-1} \Theta_{[1:l],[l+1:q]}$ . From Lemma 3.1 we know that this is equal to  $(B_{[l+1:q],[l+1:q]})^{-1}$ . Now, by the same argument as in Theorem 3.38, it follows that

$$\left\| (B_{[l+1:q],[l+1:q]})^{-1} \right\| \leq CH^{2l} J^{(l+1),-1}$$

□

This immediately provides us with a bound for the low rank approximation error, in the setting of Theorem 3.42:

**Corollary 3.57.** *Under the conditions of Theorem 3.42, we have  $\|L^{(l)} L^{(l),T} - \Gamma\| \leq Ch^{2l(s-d/2)}$ .*

## 4 Implementation and Numerical Results

The scripts and Matlab functions that were used to create the numerical experiments described in this paper can be found at

<https://github.com/f-t-s/nearLinKernel.git>

### 4.1 Tracking the sparsity pattern

Our focus will be on the analysis of the mathematical phenomena leading to exponentially localised Cholesky factors rather than the details of numerical implementation. There are multiple ways of keeping track of the sparsity pattern from a given set of measurement locations and our purpose is to describe one of them as a possible efficient implementation of the algorithm.

Let  $\{x_i\}_{1 \leq i \leq N} \subset [0, 1]^2$ , be a set of measurement locations, such that  $\max_{x \in [0, 1]^2} \min_{1 \leq i \leq N} |x_i - x| \leq 2^{q+2}$  and  $\min_{1 \leq i \neq j \leq N} |x_i - x_j| \geq \delta_{\text{mesh}} 2^q$ . let  $G$  be the Green's function of an elliptic partial differential equation of order  $2s$ , with  $s > 1$  on a domain  $\Omega'$  such that  $[0, 1]^2 \subset \subset \Omega'$ . We assume that we are given access to  $\Theta_{i,j} := G(x_i, x_j)$  and  $x_i$  and wish to compute a permutation  $P$  and a sparse Cholesky factor  $L$  such that  $P\Theta P^T \approx LL^T$ . In the following,  $\rho$  will be the accuracy parameter of our algorithm. By recursive quadratic subdivision of subregions of  $[0, 1]^2$  into four quadratic regions of half the original size, one obtains for each  $k$  a family  $\{\Omega_i^{(k)}\}_{\tilde{j}^{(k)}}$  of quadratic subregions (we will, for notational convenience, avoid being explicit about the *open/closed interval decision*). Now we introduce a graph with a vertex set  $G$  consisting of elements of  $I \cup \{0\} \times J \times \mathbb{R}$  and two sets of directed edges,  $T$  and  $E$ . Initialising it with a single vertex  $(0, 0, 0)$  and initialising  $\tilde{I}$  as  $I := [1, \dots, N]$ , we construct  $G$  as follows:

Starting from  $k = 1$ , for every  $j \in \{j \in \tilde{J}^{(k)} \mid \text{for some } 1 \leq i \leq N, x_i \in \Omega_j^{(k)}\}$  we add a vertex  $(0, j, 0)$ . For all vertices  $g, h \in G$  that we added on this level, we add the edge  $(g, h)$  to  $E$ , if the distance between the corresponding subdomains is upper bounded by  $\rho 2^{-k}$ . We furthermore add the edge  $(g, h)$  to  $T$ , if  $g$  and  $h$  correspond to subdomains  $j$  and  $\tilde{j}$  on consecutive levels, such that  $j \subset \tilde{j}$ . Finally, for each new  $g$  corresponding to the subdomain closest to the origin, (the *lower left element of the subdivision*), if it contains any  $x_i$  for  $i \in J$ , we set the second component of its parent w.r.t.  $T$  to  $i$  and remove  $i$  from  $I$ . We proceed this way, until  $I$  is empty. Now, for every element  $i \in I$ , there exists a vertex  $g$  such that its first component is equal to  $i$ . We denote this vertex by  $g_i$ . On the vertices each level of  $G, T$ , we introduce an arbitrary ordering,  $\prec^{(k)}$ . Now, for every  $i \in I$ , we define

$$G_i := \left\{ h \in \text{desc}_{(G, E)} \mid g_i \prec^{(k)} h \right\} \cup \left( \bigcup_{h \in \text{desc}_{(G, E)}} \text{desc}_{(G, T)} \right)$$

and define  $V_i, T_i$  as a copy of  $(G, T)$  restricted to  $G_i$ . For the copy of  $g_j$  in  $V_i$ , we set its third component to  $\Theta_{i,j}$ .

The above data structure can be constructed with a minor variation of the quadtree algorithm of Wendland (2005) in  $\mathcal{O}(\rho^d N \log(N))$ . Setting  $J^{(k)}$  as those elements  $i \in I$  such that  $g_i$  is on level  $k$  of the quadtree, we can check that the sampling strategy thus implied fulfils the requirements of our theorems. By passing in parallel through  $V_j, E_j$  and the corresponding subgraph of  $V_i$ , the sparsity pattern in the inner loop of Algorithm 6 can be tracked efficiently.

For our numerical experiments, we will use the Matérn family of covariance kernels:

### 4.2 The Matérn family

#### 4.2.1 Definition and properties

The Matérn family of kernels, originally introduced by Matérn (1960), is a family of kernels used in many branches of statistics and machine learning to model random fields different, finite, order of smoothness (Guttorp and Gneiting, 2006; Rasmussen and Williams, 2006). It is defined as

$$G(x, y) := \frac{2^{1-\nu}}{\Gamma(\nu)} \left( \frac{\sqrt{2\nu}|x - y|}{l} \right)^\nu K_\nu \left( \frac{\sqrt{2\nu}|x - y|}{l} \right), \quad (4.1)$$

where  $K_\nu$  is the modified Bessel function of second kind (Abramowitz and Stegun, 1964, Section 9.6) and  $\nu, l$  are parameters describing the degree of smoothness, and the length scale of interactions, respectively (Rasmussen and Williams, 2006). For  $\nu = p + 1/2$ ,  $p \in \mathbb{N}$ , the Matérn kernel take a particularly simple form (Rasmussen and Williams, 2006), yielding for example:

$$G_{1/2}(x, y) = \exp\left(-\frac{|x - y|}{l}\right) \quad (4.2)$$

$$G_{3/2}(x, y) = \left(1 + \sqrt{3}\frac{|x - y|}{l}\right) \exp\left(-\frac{\sqrt{3}|x - y|}{l}\right) \quad (4.3)$$

$$G_{5/2}(x, y) = \left(1 + \sqrt{5}\frac{|x - y|}{l} + 5\frac{|x - y|^2}{l^2}\right) \exp\left(-\frac{\sqrt{5}|x - y|}{l}\right). \quad (4.4)$$

Stein (1999) strongly recommends the Matérn family as a model for spatial statistics for its capability to allow for small scale structure as opposed to, say, the Gaussian covariance function.

When considered as function on  $\mathbb{R}^d \times \mathbb{R}^d$ , the Fourier transform of the Matérn kernel is given by

$$\hat{G}(s) = \frac{2^d \pi^{d/2} \Gamma(\nu + d/2) (2\nu)^\nu}{\Gamma(\nu) l^{2\nu}} \left(\frac{2\nu}{l^2} + 4\pi^2 |s|^2\right)^{-(\nu + d/2)}. \quad (4.5)$$

As was observed by Whittle (1954, 1963), this makes the Matérn kernel the Green's function of (possibly fractional) order  $2(\nu + d/2)$ . Accordingly, the Matérn kernel has found uses in meshfree methods for PDEs (Schaback, 2007; Cockayne et al., 2016; Raissi et al., 2017b) and Bayesian inverse problems involving PDEs (Dunlop et al., 2016; Roininen et al., 2014).

Recently it has been observed that in large applications, featuring a simple low dimensional geometry, for example the surface of the earth in spatial statistics, it can be beneficial to work directly with the underlying PDE. While it is conceptually more difficult to solve a PDE than to evaluate a closed form formula, merely writing down the kernel matrix will require  $\mathcal{O}(N^2)$  operations, where  $N$  is number of measurement points. Writing down the discretised precision operator, on the other hand, requires  $\mathcal{O}(n)$  operations, where  $n$  is the number of degrees of freedom used for the discretisation. The computation of a Cholesky factorisation, which is needed to sample from the gaussian process, then requires  $\mathcal{O}(N^3)$  time- and  $\mathcal{O}(N^2)$  space-complexity when working with the kernel matrix. If the spatial dimension is  $d = 2$ , Cholesky factorisation of the precision matrix requires only  $\mathcal{O}(n^{3/2})$  time- and  $\mathcal{O}(n \log(n))$  space complexity, by using a nested dissection ordering. Based on this reasoning, Lindgren et al. (2011) proceed by directly constructing the precision matrix as a discretised elliptic PDE and thus obtain an algorithm with complexity  $\mathcal{O}(n^{3/2})$  in time and  $\mathcal{O}(n \log(n))$  in space. A similar approach has been used in Roininen et al. (2014), in the context of inverse problems motivated by electric impedance tomography. Hou and Zhang (2017) propose to use this link between Matérn kernels and elliptic PDE to perform a sparse PCA of the Matérn covariance operator by using a generalisation of the *gamblets* of Owhadi (2017) to higher-dimensional elliptic operators (obtained independently of Owhadi and Scovel (2017)). One shortcoming of the above mentioned PDE based methods is that they are much more difficult to apply in the case where the kernel has fractional order of smoothness (that might also be spatially varying), since they require an explicit discretisation of the underlying PDE. This is a downside, since one of the attractions of the Matérn model class is the ability to continuously vary the smoothness assumption. While our theoretical results only encompass even integer order elliptic PDE, the algorithm itself does not require any prior knowledge of the order of the PDE. Indeed, our numerical examples show the same behaviour for the fractional case, as illustrated in Section 4.3.6.

We note that the Matérn kernel sampled on points in  $[0, 1]^2$  is not, strictly speaking, covered by our theoretical results. This is due to the fact that the Matérn kernels are Green's functions for the whole space, whereas our measurements are contained in a bounded domain. Correspondingly, while our kernel approximations close to the boundary are visually indistinguishable from the true kernel, the exponential decay of conditional covariances among boundary points does not decay up to scale. We have documented these artifacts in Section 4.3.5.

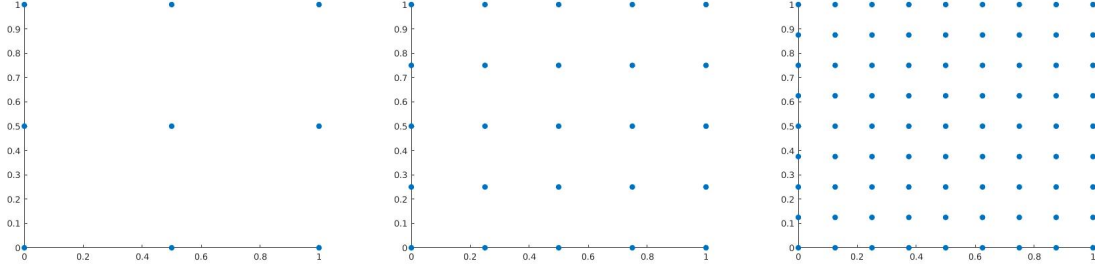


Figure 8: Configuration of points on different scales: These plots show the positions of the  $x_i$  on the first three levels, without perturbation.

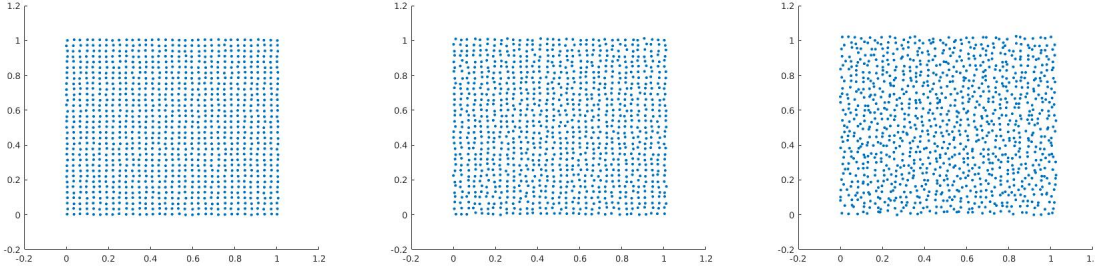


Figure 9: Different levels of perturbation: These plots show the positions of the  $x_i$  after perturbation for  $q = 5$  and  $\delta_x = \{0.1, 0.2, 0.4\}$

### 4.3 Numerical experiments

#### 4.3.1 The basic set-up

For our numerical experiments we use the domain  $[0, 1]^2$  and a uniform grid of points created by  $q$  subdivisions of the domain, as indicated by Figure 8. We use this regular grid only for the ease of implementation. In order to show that regularity of the grid it is not necessary for our algorithm to work, we introduce in each dimension a random perturbation of  $2^{-q}\delta_x \text{UNIF}(-1, 1)$ , for  $q$  the number of levels. For  $q = 5$ , the effect of this perturbation is shown in Figure 9. Ordering the points  $x_i$  from points on coarse levels to points on finer ones, we obtain our covariance matrix matrices  $\Gamma$  as

$$\Gamma_{i,j} := \frac{2^{1-\nu}}{\Gamma(\nu)} \left( \frac{\sqrt{2\nu}|x_i - y_j|}{l} \right)^\nu K_\nu \left( \frac{\sqrt{2\nu}|x_i - y_j|}{l} \right). \quad (4.6)$$

For a tuning parameter  $\rho$ , we consider the sparsity set  $S := S_\rho := \{(i, j) \text{ s. t. } \|x_i - x_j\| \leq \rho 2^{\min(\text{lev}(i), \text{lev}(j))}\}$ , where  $\text{lev}(i)$  is the smallest  $k$  such that  $i \in I^{(k)}$ . In Figure 10, the interactions of points on different levels are visualised. The sparsified kernel matrix  $\tilde{\Gamma}^\rho$  is then obtained from  $\Gamma$  by setting all entries that are not in  $S_\rho$ , to zero. The sparse Cholesky factor  $L^\rho$  is then obtained by applying the matlab function “ichol” with option “nofill” to  $\tilde{\Gamma}^\rho$ , which performs an incomplete Cholesky decomposition, which is equivalent to Algorithm 6. Finally, the resulting approximation of the kernel is obtained as  $\Gamma^\rho := L^\rho L^{\rho,T}$ . The numerical results presented here are simple illustrative examples of our theoretical results obtained from artificially created measurement points. We plan to develop a fully sparsity exploiting implementation of our algorithm as a follow up project and use it to analyse the performance of our method for problems that are too large to be treated with dense linear algebra.

#### 4.3.2 Compression factors and relative errors

As a first step, we will report on the compression ratios and relative approximation errors obtained by our method. We start out, by considering the Matérn kernel with smoothness  $\nu = 1$  and length scale of

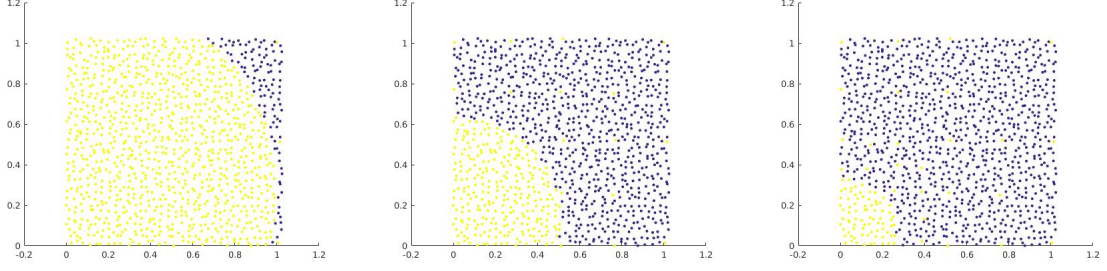


Figure 10: Range of interaction: For points  $x_i$  on level 2 , 3 and 4, the set  $\{x_j \text{ s.t. } (i, j) \in S_2\}$  is marked in yellow.

$\rho$	$\ \Gamma^\rho - \Gamma\ $	$\ \Gamma^\rho - \Gamma\ /\ \Gamma\ $	$\ \Gamma^\rho - \Gamma\ _{\text{Fro}}$	$\ \Gamma^\rho - \Gamma\ _{\text{Fro}}/\ \Gamma\ _{\text{Fro}}$	$\#S$	$\#S/N^2$
2.0	2.415e+00	8.689e-04	7.863e+00	5.712e-04	5.229e+06	1.888e-02
4.0	2.391e-02	8.602e-06	9.244e-02	5.655e-06	1.528e+07	5.519e-02
6.0	1.259e-03	4.529e-07	4.966e-03	2.978e-07	2.777e+07	1.003e-01
8.0	2.664e-04	9.585e-08	1.103e-03	6.301e-08	4.166e+07	1.504e-01
10.0	8.991e-05	3.235e-08	3.688e-04	2.127e-08	5.601e+07	2.023e-01
12.0	3.628e-05	1.305e-08	1.459e-04	8.580e-09	7.086e+07	2.559e-01
14.0	1.649e-05	5.933e-09	7.058e-05	3.900e-09	8.578e+07	3.098e-01

Table 1: Compression and accuracy for  $q = 7$ ,  $l = 0.2$ ,  $\nu = 1$ ,  $\delta_x = 0.2$  and different values of  $\rho$ .

interaction  $l = 0.2$ . For these values, the Matérn kernel corresponds to the Greens function of an elliptic operator of order 4. In Table 1, we show the resulting absolute and relative error in Frobenius- and operator norm and the compression ratio compared to a dense matrix, for different values of  $\rho$ . To show that even very long correlation length do not lead to a breakdown of our method, we try the same kernel but this time with an interaction length of  $l = 0.4$ . As one can see in Table 2, for a given  $\rho$ , we get similar approximation properties as in the first example. As a next example we will take again  $l = 0.2$  but we will take  $\nu = 2$ . This corresponds to the Green's operator of an elliptic equation of order 6. This time, the minimal value of  $\rho$  that we have to choose is larger, larger condition number has to be compensated for by a decrease in truncation error. We compile our result in Table 3. In Figure 11 we have plotted the relative error in operator norm on a logarithmic scale. The first panel shows the error obtained over the entire domain. For small relative accuracy we observe a saturation of the exponential decay, which we attribute to the boundary effects discussed in Section 4.3.5. The second panel shows the relative error in operator norm of the approximation of  $\hat{\Gamma}$  by  $\hat{\Gamma}^\rho$ , where  $\hat{\cdot}$  denotes the restriction to entries  $(i, j)$  such that  $x_i, x_j \in [0.1, 0.9]^2$ . As we can see from the second panel of Figure 11, the exponential decay of the error in the interior of the domain is more rapid and is not subject to this saturation effect.

$\rho$	$\ \Gamma^\rho - \Gamma\ $	$\ \Gamma^\rho - \Gamma\ /\ \Gamma\ $	$\ \Gamma^\rho - \Gamma\ _{\text{Fro}}$	$\ \Gamma^\rho - \Gamma\ _{\text{Fro}}/\ \Gamma\ _{\text{Fro}}$	$\#S$	$\#S/N^2$
2.0	2.048e+00	3.167e-04	5.658e+00	2.774e-04	5.228e+06	1.888e-02
4.0	1.871e-02	2.893e-06	5.920e-02	2.535e-06	1.528e+07	5.518e-02
6.0	2.452e-03	3.792e-07	6.626e-03	3.322e-07	2.776e+07	1.002e-01
8.0	3.647e-04	5.639e-08	1.389e-03	4.941e-08	4.166e+07	1.504e-01
10.0	1.573e-04	2.431e-08	5.603e-04	2.130e-08	5.601e+07	2.023e-01
12.0	7.186e-05	1.111e-08	2.361e-04	9.734e-09	7.085e+07	2.559e-01
14.0	3.081e-05	4.764e-09	9.432e-05	4.174e-09	8.578e+07	3.098e-01

Table 2: Compression and accuracy for  $q = 7$ ,  $l = 0.4$ ,  $\nu = 1$ ,  $\delta_x = 0.2$  and different values of  $\rho$ .

$\rho$	$\ \Gamma^\rho - \Gamma\ $	$\ \Gamma^\rho - \Gamma\ /\ \Gamma\ $	$\ \Gamma^\rho - \Gamma\ _{\text{Fro}}$	$\ \Gamma^\rho - \Gamma\ _{\text{Fro}}/\ \Gamma\ _{\text{Fro}}$	$\#S$	$\#S/N^2$
6.0	1.249e-02	4.220e-06	3.910e-02	2.687e-06	2.776e+07	1.003e-01
8.0	1.170e-04	3.953e-08	6.446e-04	2.517e-08	4.166e+07	1.505e-01
10.0	1.861e-05	6.287e-09	9.154e-05	4.003e-09	5.601e+07	2.023e-01
12.0	3.492e-06	1.180e-09	1.521e-05	7.511e-10	7.086e+07	2.559e-01
14.0	7.798e-07	2.634e-10	3.659e-06	1.677e-10	8.578e+07	3.098e-01

Table 3: Compression and accuracy for  $q = 7$ ,  $l = 0.2$ ,  $\nu = 2$ ,  $\delta_x = 0.2$  and different values of  $\rho$ .

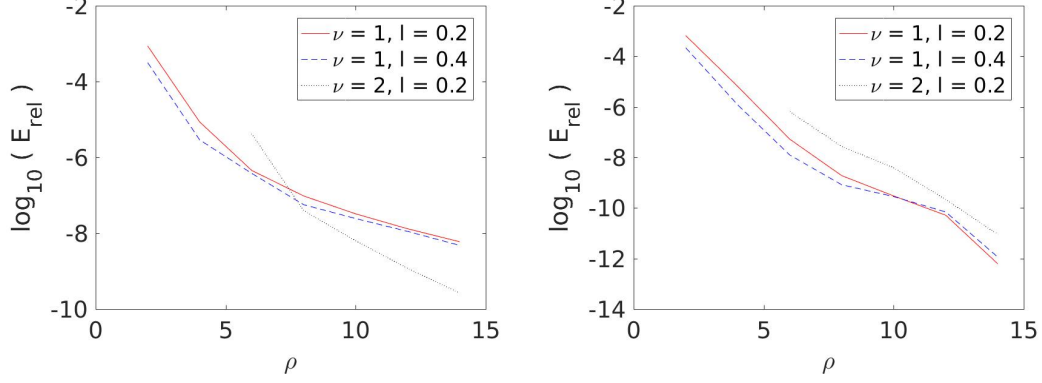


Figure 11: Exponential decay of error: We see plotted, for the three kernels considered in Section 4.3.1, the decay of the relative error in operator norm as  $\rho$  increases. The first panel shows the error made over the entire domain. The second considers the relative error made on the submatrix corresponding to sampling points in  $[0.1, 0.9]^2$ .

#### 4.3.3 Truncated versus incomplete factors

The only obstacle in providing error estimates for Algorithm 6 is that we were so far not able to rigorously bound the difference between the approximation obtained from the Cholesky factors  $L^\rho$ , which are computed by Algorithm 8, and the approximation obtained by computing the exact Cholesky factor  $L$  and then approximating  $\Gamma$  by  $(L|_S)(L|_S)^T$ . The size of this effect, compared to the approximation error when truncating the exact Cholesky factors, is tabulated in Tables 4, 5 and 6 for the kernels investigated in Section 4.3.1. We see that the difference between the approximation obtained by Algorithm 6 and the truncation of the exact Cholesky factors is bounded from above by the approximation error incurred when using the truncation of the exact Cholesky factors, throughout our experiments. This provides strong numerical evidence that Algorithm 6 actually provides us with a simple, near linear complexity algorithm.

#### 4.3.4 Irregularity of the grid and points on a submanifold

In this section we want to investigate the robustness of our algorithm to the placement of the sampling points  $x_i$ . Recall that our set of sampling points is initially generated as a uniform grid, which is then subject to random perturbations of magnitude  $\delta_x 2^{-q}$ . In the last section, we choose  $\delta_x$  to be 0.2,

$\rho$	2.0	4.0	6.0	8.0	10.0	12.0	14.0
$\ L^\rho L^{\rho,T} - (L _S)(L _S)^T\ $	5.278e+00	6.671e-02	3.051e-03	5.030e-04	1.404e-04	5.183e-05	2.163e-05
$\ (L _S)(L _S)^T - \Gamma\ $	8.926e+00	1.085e-01	5.753e-03	1.228e-03	4.012e-04	1.570e-04	7.474e-05
$\frac{\ L^\rho L^{\rho,T} - (L _S)(L _S)^T\ }{\ (L _S)(L _S)^T - \Gamma\ }$	5.913e-01	6.147e-01	5.304e-01	4.098e-01	3.499e-01	3.301e-01	2.894e-01

Table 4: Error induced by the incomplete factorisation for  $q = 7$ ,  $l = 0.2$ ,  $\nu = 1$ ,  $\delta_x = 0.2$  and different values of  $\rho$ .

$\rho$	2.0	4.0	6.0	8.0	10.0	12.0	14.0
$\ L^\rho L^{\rho,T} - (L _S)(L _S)^T\ $	4.209e+00	4.040e-02	4.459e-03	5.787e-04	2.326e-04	9.249e-05	3.512e-05
$\ (L _S)(L _S)^T - \Gamma\ $	6.832e+00	6.992e-02	7.920e-03	1.520e-03	6.140e-04	2.574e-04	1.018e-04
$\frac{\ L^\rho L^{\rho,T} - (L _S)(L _S)^T\ }{\ (L _S)(L _S)^T - \Gamma\ }$	6.161e-01	5.779e-01	5.630e-01	3.807e-01	3.789e-01	3.593e-01	3.450e-01

Table 5: Error induced by the incomplete factorisation for  $q = 7$ ,  $l = 0.4$ ,  $\nu = 1$ ,  $\delta_x = 0.2$  and different values of  $\rho$ .

$\rho$	6.0	8.0	10.0	12.0	14.0
$\ L^\rho L^{\rho,T} - (L _S)(L _S)^T\ $	3.908e-02	6.520e-04	9.081e-05	1.393e-05	2.625e-06
$\ (L _S)(L _S)^T - \Gamma\ $	4.907e-02	8.555e-04	1.197e-04	1.944e-05	4.442e-06
$\frac{\ L^\rho L^{\rho,T} - (L _S)(L _S)^T\ }{\ (L _S)(L _S)^T - \Gamma\ }$	7.965e-01	7.622e-01	7.584e-01	7.167e-01	5.909e-01

Table 6: Error induced by the incomplete factorisation for  $q = 7$ ,  $l = 0.2$ ,  $\nu = 2$ ,  $\delta_x = 0.2$  and different values of  $\rho$ .

which destroys the simple regular structure of the initial mesh but still prevents neighbouring points from coming too close together. In this section we are going to drastically increase the size of the perturbation, thus creating highly irregular point clouds. We will choose values of  $\delta_x \in \{0.2, 0.4, 2, 4\}$  for a kernel with  $\nu = 1$  and  $l = 0.2$ . In Figure 12, the corresponding point clouds are plotted. In Table 7, we tabulated the resulting approximation error for  $\rho = 6$ . Note that for  $\delta_x \in \{0.2, 0.4\}$ , a lower bound on  $\delta_{\text{mesh}}$  as in Examples 3.32 3.34 and 3.33 is still guaranteed. For  $\delta_x \in \{2, 4\}$ , instead, very tight clustering of measurement points can occur. We note that under inclusion of moderate irregularity the accuracy of the approximation is more or less stable or even improving slightly. When increasing the perturbation to  $\delta_x = 4$ , we have the first notable, although small deterioration of accuracy. This however goes along with a small decrease in the size of  $\#S$ , making the *net-deterioration*, after accounting for the decrease of  $\#S$ , even smaller. Since the choice of the ordering in our implementation happens before the perturbation is applied, this simultaneously shows robustness of the algorithm under the choice of the multiresolution ordering. One advantage of using covariance kernels, as opposed to an explicit discretisation of the underlying PDE, is that kernel based methods adapt nicely to points that do not lie exactly in a low dimensional Euclidean space, but instead might be clustered around a low dimensional submanifold of a higher dimensional space. In order to test, how our method deals with this situation, we use introduce a new parameter  $\delta_z$ , and add to every point  $x_i \in \mathbb{R}^2$  a third component

$$x_i^{(3)} := -\delta_z \sin\left(6x_i^{(1)}\right) \cos\left(2x_i^{(2)}\right) + 2\delta_x 2^{-q} \delta_z \epsilon_i^{(3)}, \quad (4.7)$$

where the  $\epsilon_i^{(3)} \sim \text{UNIF}(-1, 1)$  independent rando variables. In Figure 13, we plot the thus obtained point clouds of  $q = 7$ ,  $\delta_x = 2$  and  $\delta_z \in \{0, 0.1, 0.2, 0.4\}$ . Using these sets of sampling points, for a Matérn kernel with  $\nu = 1$  and  $l = 0.2$ , we obtain the numerical results summarised in Table 8. We see that while there is a mild increase in approximation error, as  $\delta_z$  is increased, we overall obtain a good approximation even for  $\delta_z = 0.4$ , when  $z$ -axis variability is almost as large as  $x$ - and  $y$ -axis variability. We further note that because of the increasing distance between points,  $\#S$  is also decreasing. If one were to compensate for this decrease by slightly decreasing  $\rho$ , the *net-deterioration* would be even smaller.

$\delta_x$	$\ \Gamma^\rho - \Gamma\ $	$\ \Gamma^\rho - \Gamma\ /\ \Gamma\ $	$\ \Gamma^\rho - \Gamma\ _{\text{Fro}}$	$\ \Gamma^\rho - \Gamma\ _{\text{Fro}}/\ \Gamma\ _{\text{Fro}}$	$\#S$	$\#S/N^2$
0.2	4.336e-03	1.560e-06	1.669e-02	1.026e-06	2.125e+07	7.675e-02
0.4	4.495e-03	1.617e-06	1.706e-02	1.063e-06	2.128e+07	7.683e-02
2.0	4.551e-03	1.638e-06	1.820e-02	1.077e-06	2.127e+07	7.682e-02
4.0	8.158e-03	2.940e-06	2.976e-02	1.933e-06	2.119e+07	7.652e-02

Table 7: Compression and accuracy for  $q = 7$ ,  $l = 0.2$ ,  $\rho = 5$ ,  $\nu = 1$  and different values of  $\delta_x$ .



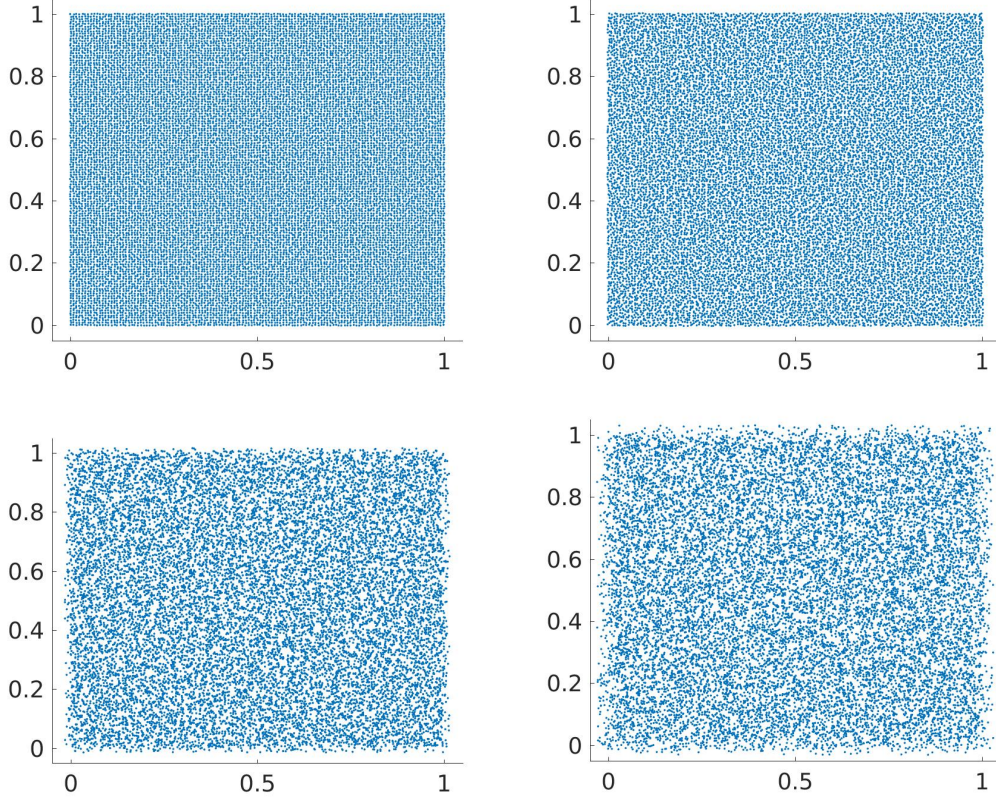


Figure 12: Different degrees of perturbation: The above plots show the measurement points  $x_i$  for  $q = 7$  and  $\delta_x = \{0.2, 0.4, 2, 4\}$

$\delta_z$	$\ \Gamma^\rho - \Gamma\ $	$\ \Gamma^\rho - \Gamma\ /\ \Gamma\ $	$\ \Gamma^\rho - \Gamma\ _{\text{Fro}}$	$\ \Gamma^\rho - \Gamma\ _{\text{Fro}}/\ \Gamma\ _{\text{Fro}}$	$\#S$	$\#S/N^2$
0.0	5.049e-03	1.560e-06	1.885e-02	1.026e-06	2.126e+07	7.677e-02
0.1	6.341e-02	1.648e-06	1.232e-01	1.077e-06	2.083e+07	7.521e-02
0.2	1.204e-01	1.749e-06	2.203e-01	1.126e-06	1.976e+07	7.137e-02
0.4	1.954e-01	3.550e-06	5.098e-01	2.197e-06	1.722e+07	6.218e-02

Table 8: Compression and accuracy for  $q = 7$ ,  $l = 0.2$ ,  $\rho = 5$ ,  $\nu = 1$ ,  $\delta_x = 2$  and different values of  $\delta_z$ .

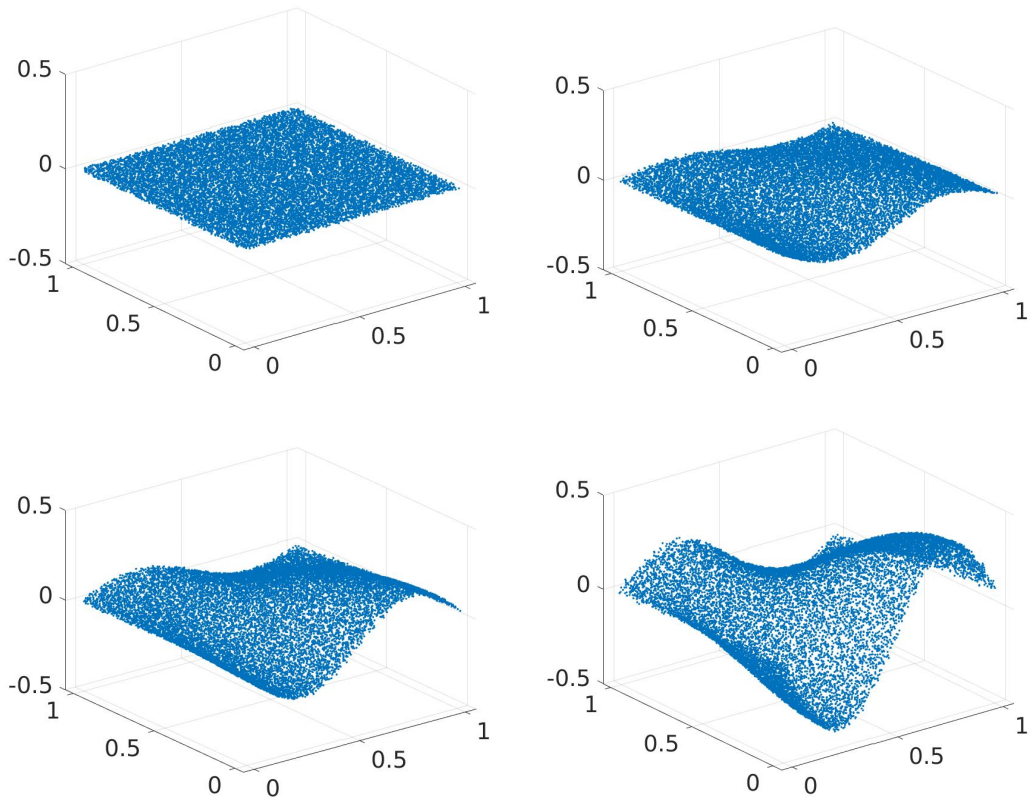


Figure 13: Different amounts of vertical variability: The above plots show the measurement points  $x_i$  for  $q = 7$ ,  $\delta_x = 2$  and  $\delta_z \in \{0, 0.1, 0.2, 0.4\}$

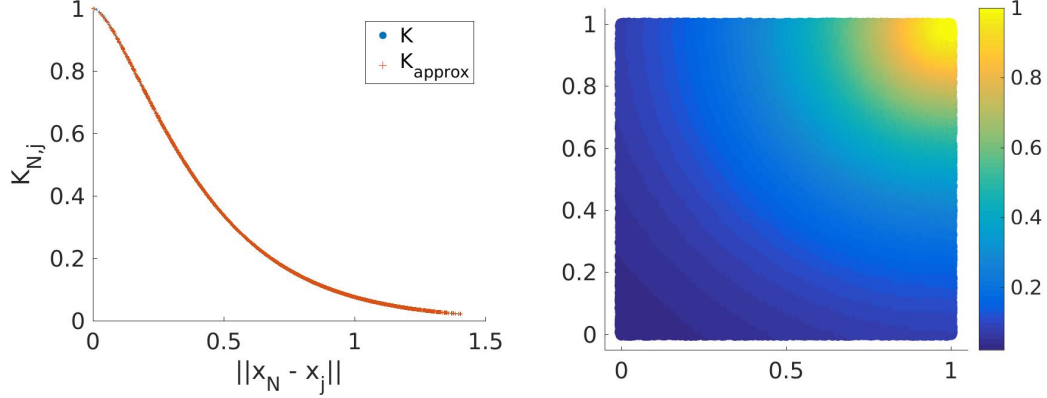


Figure 14: Accurate representation of a boundary point: The first panel shows the values of the true and the approximate kernel based in  $x_N$ , the last point of the ordering. The second panel shows the value of the approximate kernel based in this point, in the physical domain.

#### 4.3.5 Detoriation of exponential decay at the boundary

Unfortunately, the Matérn family is not covered by our theoretical guarantees since it corresponds to a Green’s function on the whole space, whereas our measurement points are only dense in a bounded subset of  $\mathbb{R}^2$ . PDE based methods for representing the Matérn kernels, as those of Lindgren et al. (2011) and Roininen et al. (2014) need to specify boundary conditions, so that the partial differential operators has a unique inverse. As noted by Roininen et al. (2014) this choice can severely affect the resulting covariance operator, with Dirichlet– or Neumann boundary conditions leading to an under– or overestimation of the covariances close to the boundary. Roininen et al. (2014) observe that Robin boundary conditions with a well chosen coefficient can yield a much better approximation of the Matérn covariance operator. Furthermore it is noted that an artificial extension of the computational domain can decrease the effect of boundary conditions. Daon and Stadler (2016) treat the problem of mitigating the boundary effects in PDE based approaches to Gaussian processes in more detail. The authors present methods based on the optimal choice of coefficients of the Robin boundary conditions and the normalisation of the variance to decrease the influence of the boundary conditions of the covariance operator.

In contrast to these observations, the approximate covariance kernel obtained by our method is visually indistinguishable from the true covariance kernel, without any need from the side of the user to specify boundary conditions. This is shown in illustrated in Figure 14, where the covariances of a point in a corner of the domain are plotted. For this figure, we have chosen a large lengthscale  $l = 0.4$  and a small compression ratio  $\rho = 2$ , in order to maximise the effects caused by the finiteness of  $\Omega = [0, 1]^2$ . In the first panel of Figure 14, the value of the exact and approximate kernel is plotted against the distance of the evaluation points. In the second panel, the value of this kernel approximation is visualised in the physical domain.

While we do get very good approximation results even at the boundary, asymptotic decay of correlations does not happen to the same extent as in the inside of the domain. To illustrate this, the first panel of Figure 15 plots the  $i$ -th column of the Cholesky factor  $L$  of  $K$  for an  $x_i$  in the interior of the domain. The second panel of Figure 15 plots the  $j$ -th column of  $L$  for an  $x_j$  on the same level, on the boundary. The appearance of these residual long range correlations among boundary points, which appears particularly strongly if the lengthscale of interaction is large, compared to the size of the domain, is not surprising. After all, our method is based on the screening effect and there are no measurements outside of  $[0, 1]^2$  on which we can condition to prevent communication between boundary points. While this might limit the performance of our method in the regime of very long interactions, there are a number of remedies to this problem.

1. First, the number of boundary points is relatively small. Therefore, it is possible to include interactions among boundary points on a longer scale than interactions involving interior points, for only a small increase of algorithmic complexity. Furthermore, one might want to include more boundary

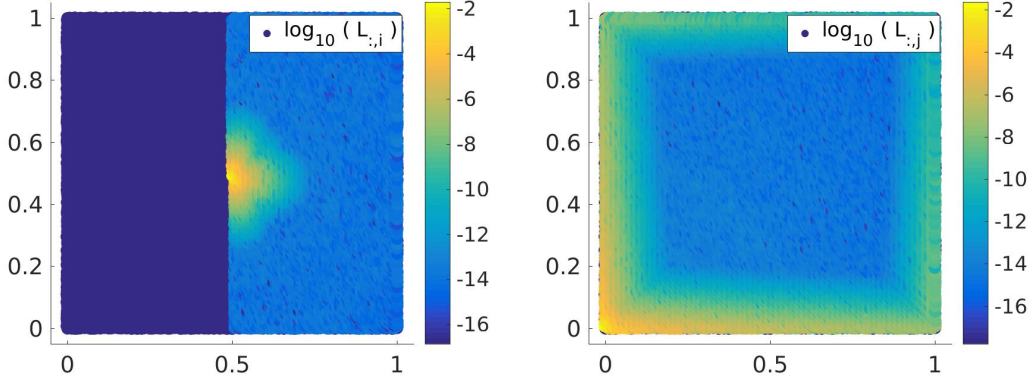


Figure 15: Strong interactions among boundary points: The first panel shows the  $i$ -th column of the Cholesky factor  $L$  of  $K$  (with  $\nu = 1$ ,  $l = 0.4$  for an  $x_i$  in the interior of the domain. The second panel shows the  $j$ -th column of  $L$  for a  $x_j$  on the lower, left corner of domain. Both  $x_i$  and  $x_j$  are on the finest level of the hierarchy. The all zero region in the first panel is caused by the elimination of these variables in the Cholesky factorisation.

points on the coarser scales, in order to increase the screening effect among boundary points. In our experiments, our measurement points are chosen with a high, constant density on the interior of the domain. In some applications, it is to be expected that the density of measurement points will decrease towards the boundary of the domain. In such a situation, by including with each level of the hierarchy an entire layer of boundary points, starting from the outer layers, one might be able to induce a stronger screening effect among measurements on the boundary.

2. We note that the results shown in the second panel of Figure 11 indicate that on the slightly smaller subdomain  $[0.1, 0.9]^2$  the effect of the boundary has already diminished drastically. In applications where one has access to the covariance function it is possible to introduce artificial measurement points on the boundary, in order to induce a stronger screening effect on the variables on the boundary of the domain. By making the former boundary of the domain of measurement part of the interior of an extended domain, a very accurate approximation of their covariances can be obtained. This approximation can then be used to apply the matrix  $\Theta$  in near linear time, or generate normal random variables with covariance  $\Theta$ . To apply the inverse of the covariance matrix, the highly accurate sparse approximation of  $\Theta$  obtained by the artificial measurements can be inverted using the conjugate gradient method, with the approximation  $\Theta^\rho$ , as obtained without artificial measurements, serving as a preconditioner.
3. What is the statistical meaning of  $\Theta^\rho$ ? The weak, long range correlations among boundary points correspond to an implicit estimate of gaussian process outside of the domain of measurement. Depending on the context, these estimates might not be very reliable, thus the truncation of these correlations might actually be sensible, from a statistical point of view. In particular we note that our approximate covariance kernel does not exhibit the boundary artifacts described by Roininen et al. (2014) and Daon and Stadler (2016). On this note, it might be interesting to compare the boundary values produced by our method with the optimal robin boundary conditions identified by Daon and Stadler (2016)

#### 4.3.6 Fractional operators

For any given dimension  $d$ , for almost all values of  $\nu$ , the corresponding PDE will not be of integer order, but contain fractional derivatives. For PDE based methods that rely on the explicit discretisation of the partial differential operators, such as those of Lindgren et al. (2011), Hou and Zhang (2017), and Roininen et al. (2014), the treatment of fractional orders results in additional difficulties, both theoretically and in terms of the implementation. Our algorithm does not explicitly discretise the differential operator, it is

$\nu$	$\ \Gamma^\rho - \Gamma\ $	$\ \Gamma^\rho - \Gamma\ /\ \Gamma\ $	$\ \Gamma^\rho - \Gamma\ _{\text{Fro}}$	$\ \Gamma^\rho - \Gamma\ _{\text{Fro}}/\ \Gamma\ _{\text{Fro}}$	$\#S$	$\#S/N^2$
1.0	1.266e-03	4.556e-07	4.987e-03	2.995e-07	2.776e+07	1.003e-01
1.1	1.813e-03	6.423e-07	6.216e-03	4.190e-07	2.776e+07	1.003e-01
1.3	3.235e-03	1.129e-06	1.039e-02	7.312e-07	2.776e+07	1.003e-01
1.5	5.245e-03	1.811e-06	1.652e-02	1.166e-06	2.776e+07	1.003e-01
1.6	6.800e-03	2.333e-06	2.148e-02	1.498e-06	2.776e+07	1.003e-01
1.8	9.891e-03	3.362e-06	3.088e-02	2.147e-06	2.776e+07	1.003e-01
2.0	1.238e-02	4.180e-06	3.892e-02	2.662e-06	2.776e+07	1.003e-01

Table 9: Compression and accuracy for  $q = 7$ ,  $l = 0.2$ ,  $\rho = 6$ ,  $\delta_x = 0.2$  and different values of  $\nu$ .

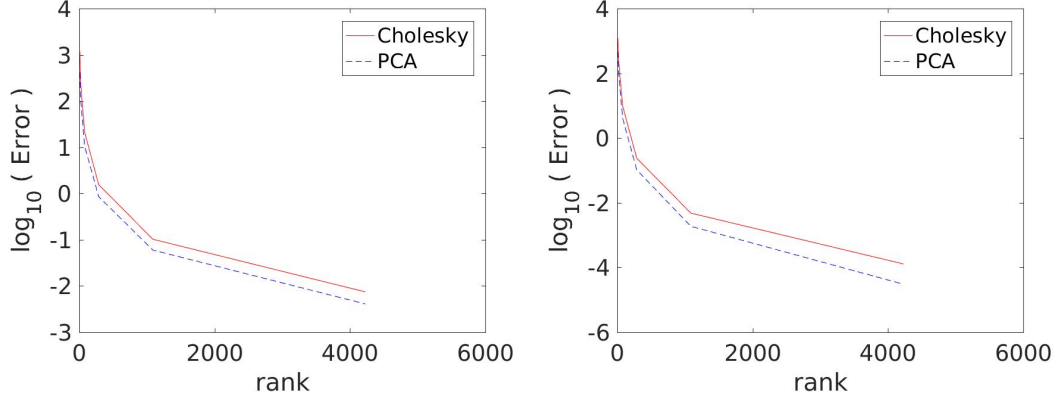


Figure 16: Near optimal sparse PCA: This figure compares the approximation ratio of the sparse PCA obtained via the restricted Cholesky decomposition with the optimal low rank approximation obtained by an eigendecomposition. In the first pane, a kernel with  $\nu = 1$ ,  $l = 0.2$ ,  $\delta_x = 0.2$  and  $\rho = 6.0$  was used. In the second panel, a kernel with  $\nu = 2$ ,  $l = 0.2$  and  $\delta_x = 0.2$  and  $\rho = 8$  was used.

entirely agnostic to its form. While our theoretical results only cover integer order operators, in Table 9, we compiled the numerical results for the Matérn kernels interpolating between PDEs of order 4 and 6. As compiled in the table, we observe very similar approximation properties for both fractional and integer order PDE. As expected the approximation ratios of the fractional Matérn kernels interpolate between the approximation ratios of the integer order kernels.

#### 4.3.7 Sparse approximate PCA

As mentioned in Section 3.7, the factorisation obtained from Algorithm 6 also implies a sparse, approximate PCA. To show that this approximate PCA provides a near optimal rank- $k$  approximation of the covariance operator, we define

$$L_{i,j}^{\rho,(k)} := \begin{cases} L^{\rho}, & \text{for } j \leq \#I^{(k)} \\ 0, & \text{else} \end{cases} \quad (4.8)$$

Here,  $\#I^{(k)}$  is the number of measurement points on the levels from 1 to  $k$ . We then define the  $\Theta^{\rho,(k)} := L^{\rho,(k)} L^{\rho,(k),T}$  as the rank  $\#I^{(k)}$ -approximation implied by  $L^{\rho,(k)}$ . In Figure 16 we have plotted the approximation error in Frobenius norm of the rank  $\#I^{(k)}$  approximation obtained from PCA and restricted Cholesky decomposition. As observed in Owhadi (2017); Hou and Zhang (2017) for gamblet based PCA, the resulting low rank approximation has near-optimal approximation rate, as the rank is increased. While higher order equations pose the additional difficulty of being more ill-conditioned, their quick spectral decay is helpful for spectral approximation. By truncating the Cholesky factors obtained from Algorithm 6, one obtains a combination of a multiscale approximation based on controlling the condition numbers on each scale – and a global low rank approximation based on the decay of the eigen-



values. From a practical point of view, this gives us a way to *salvage* a restricted Cholesky algorithm that encounters a zero pivot, because of a choice of  $\rho$  that was too small for the given kernel. In this case, the columns of the Cholesky factor computed before the pivots became close to zero will still be a near-optimal low rank approximation of the kernel matrix.

## 5 Conclusions

### 5.1 Comparison to prior work

We will now highlight similarities and differences between our approach and three classes of existing methods, with the purpose of describing interplays and relations.

#### 5.1.1 Inducing points, predictive processes and MRA

It is remarkable that the sparsity-induced *screening effect* has been used by numerical analysts mostly when dealing with sparse matrices arising from the discretization of differential operators. For these matrices, which can be seen as corresponding to precision matrices in statistics, nested dissection orderings have provided reasonably fast solvers for low dimensional problems (George, 1973). For dense matrices representing integral equations however, we are not aware of any prior work recognising that integral operators too can have sparse Cholesky factors when making appropriate use of the *screening-effect*. In the context of *sparse approximate inverse preconditioners*, Benzi (2016) and Benzi and Tuma (2000) observe that factorised preconditioners can provide better preconditioning results for a given number of nonzero entries, than direct sparse approximations of the dense inverse matrix. This kind of preconditioner has also been discovered by Harbrecht (2012) which we will comment on in the context of wavelet methods. However, while Benzi and Tuma (2000) observe that the ordering has influences the sparsity of the inverse Cholesky factor, and that the inverse Cholesky factors of sparse, well conditioned matrices are exponentially localised, these factors are interpreted as the inverse of the Cholesky factors of the sparse matrix, to be used for preconditioning purposes. It does not seem to be observed that these factors actually correspond to the Cholesky factors of the dense inverse, that they can be computed directly by an incomplete factorisation of the dense matrix and thus serve as provide a sparse and accurate representation of the inverse matrix. In the statistics community, on the other hand, notions of *conditional sparsity* have a long history and form the basis of scalable Gaussian process methods. These methods are known as *covariance tapering* (Chilès and Delfiner, 2012), *inducing points* (Quiñero-Candela and Rasmussen, 2005; Snelson and Ghahramani, 2006), *predictive processes* (Banerjee et al., 2008), and *multi-resolution approximation* (MRA) (Katzfuss, 2016). In particular, MRA and our method have in common the idea of using successive conditioning to obtain marginals with short correlation length, which is a simple way to obtain hierarchically sparse approximations of general stochastic processes. While these methods exploit the same mathematical phenomenon that causes our Cholesky factors to be localised, they do not make the connections to the sparsity of the Cholesky factorisation of the covariance matrix. In this paper, this connection leads to a very simple algorithm based on the interplay with the established theory of sparse factorisations.

In the statistics literature rigorous bounds on the approximation error seem to play a lesser role than in numerical analysis. Oftentimes, the viewpoint of finding classes of *sparse* stochastic processes that show a similar behaviour to the usual *dense* choices is emphasised. This might stem from the fact that covariance matrices in statistics are seen as tools to analyse data, rather than as *physical models* such as the equations of physics that motivated much of the research in numerical analysis. Using techniques from (numerical) analysis, we provide rigorous estimates on the tradeoff between approximation error and computational complexity for a large class of matrices, with the purpose of (1) providing a tool for the numerical analysis of localised matrices and their inverses and (2) characterising conditions implying a *screening effect*. In doing so, we observe for example that a near optimal screening effect can be obtained by controlling the mesh constants of the grids on the different levels, without the need to *seal off* the different subregions from each other in a nested-dissection approach. This is in contrast to the suggestion of Katzfuss (2016) to prefer *knots* close to the boundary of the subdomains. In fact, this would lead to a deterioration of the mesh constant and thus of our error bounds, requiring us to rely on the nested dissection-effect, which does not lead to a near-linear time algorithm for  $d > 1$ .

### 5.1.2 Wavelet methods for integral equations

In the numerical analysis community, sparsity-oriented approaches for the treatment of integral operators have mostly been based on wavelet methods. *Vanishing moments* conditions of the wavelet basis appear to be an essential requirement for these methods. We say that a family of wavelets has  $M$  *vanishing moments* if its elements on all but the coarsest level are  $L^2$ -orthogonal to polynomials of order up to  $M-1$ . Beylkin et al. (1991) observes that the integral operators associated to pseudo differential operators decay algebraically with order  $m+1$ , according to the sparsity graph induced by the geometry of the domain. This fact leads to  $\mathcal{O}(N \log N)$  or even  $\mathcal{O}(N)$  approximation schemes. Dahmen et al. (2006) shows that by using additional adaptive compression, wavelet schemes applied to integral operators can achieve accuracy up to discretisation error in  $\mathcal{O}(N)$  computational complexity when applied to integral equations. In the wavelet community, the method closest to our approach is the  $LU$  factorisation of integral operators in wavelet bases (Gines et al., 1998). There it is observed that when computing the  $LU$  factorisation of a differential operator or its inverse, represented in a wavelet basis with  $M$  vanishing moments, the factors are algebraically localised with order  $M+1$ . Since our approach also relies on the sparsity of the Cholesky decomposition of differential and integral operators represented in a multiresolution basis, the two methods appear to be, at first glance, similar. There are, however, several important differences: In Gines et al. (1998), the localisation is algebraic and originally comes from the vanishing moments of the multiresolution basis. Then it is observed that this localisation can be *preserved* during the  $LU$ -decomposition. On the contrary, in our method we do not need the integral operator to be sparse in the multiresolution basis. Instead, our localisation is *induced* by the Cholesky decomposition. In fact Owhadi and Scovel (2017) does not require the multiresolution basis to have  $s$  vanishing moments (for an elliptic partial differential operator of order  $2s$ ) to obtain exponential decay of gamblets. Furthermore, by introducing Condition 3.37 and Theorem 3.38, we are able to obtain bounded condition numbers, and thus the exponentially localised Cholesky factorisation without any vanishing moments. The reason why this behaviour was not observed by Gines et al. (1998) lies in the fact that the Cholesky factorisation was performed from fine to coarse scales. In our results, motivated by probabilistic interpretations, we discover that although the sparse matrix should be factorised from fine to coarse scales, its dense inverse should be factorised from coarse to fine scales. As mentioned in the Section 2, this type of behaviour exists for both nested-dissection and minimal-degree ordering. The reverse ordering of a sparsity-preserving ordering for the sparse matrix  $\mathcal{L}$  will provide a sparsity-inducing ordering for the dense inverse  $\Theta$ . To the best of our knowledge the possibility of sparsity-inducing Cholesky factorisations of dense matrices has not been noted before.

Another difference between Gines et al. (1998) and our work is that the former relies on the fact that the incomplete Cholesky decomposition of a sparse matrix from fine to coarse scales is a very good approximation of the ordinary Cholesky decomposition, which is not the case when performing the Cholesky decomposition from coarse to fine scales. However, as shown here, for integral equations, the error made by approximating the true Cholesky decomposition of the truncated kernel matrix with the incomplete Cholesky factorisation computed from coarse to fine scales, cancels out with the error made by the truncation itself, up to an exponentially small term. Although (Harbrecht, 2012) also uses an incomplete Cholesky decomposition from coarse to fine scales in a wavelet basis, the resulting decomposition is only used as a preconditioner for the fast inversion of a wavelet-sparsified integral equation. In particular, the authors do not observe the exponential decay of the Cholesky decomposition. This leads to the curious situation that the incomplete Cholesky preconditioner is asymptotically a better approximation of the *true* underlying equation than the sparse approximation of the integral operator that is being inverted using this preconditioner.

### 5.1.3 Fast multipole methods and hierarchical matrices

Fast multipole methods and hierarchical matrices are popular scalable approaches for dealing with dense kernel matrices. The fast multipole method, developed by Greengard and Rokhlin (1987) in the context of many-particle simulations, is based on the observation that interactions between well separated groups of particles can be approximated by relatively few terms of the potential's multipole expansion. Using these low rank approximations over a hierarchy of scales leads to near-linear complexity algorithms.

Hierarchical matrices (Hackbusch, 1999; Hackbusch and Khoromskij, 2000; Bebendorf, 2008) can be

thought of as the algebraic abstraction of the idea underlying the fast multipole method. Here, blocks that correspond to *distant* groups of points are modeled to have low rank. Many types of matrices and their inverses have been shown to be well approximated by hierarchical matrices, notably the stiffness matrices of elliptic partial differential operators and their inverses (Bebendorf, 2007, 2016), as well as kernel matrices arising from Matérn kernels (Ambikasaran et al., 2016). It turns out that from our sparse Cholesky decomposition (and also from the decomposition proposed by Gines et al. (1998)), a hierarchical matrix type approximation of  $\Theta$  or  $A$  can be derived. This can be seen by observing that the truncated Cholesky decomposition  $L^\rho L^{\rho,T} = \Theta$  can be rewritten as  $\Theta = \sum_{i=1}^N l_i l_i^T$ , where  $l_i := L_{1:N,i}^\rho$ . Now let  $S_1, S_2 \subset I$  be two sets of indices corresponding to points in regions  $\Omega_1, \Omega_2$ , such that  $\text{diam}(\Omega_1) \approx \text{diam}(\Omega_2) \approx \text{dist}(\Omega_1, \Omega_2) \approx 2\rho h^k$ . Then, for  $i \in S_1 \cap J^{(l)}$ ,  $l > k$ , we have  $(l_i)_j = L_{i,j}^\rho = 0$ . Therefore, we have  $\#\{i \in I \mid l_i l_i^T|_{S_1 \times S_2} \neq 0\} \lesssim q\rho^d$ , where  $q$  is the number of levels and  $d$  the spatial dimension. Based on this argument, our sparse Cholesky decomposition (and equally the one of Gines et al. (1998)) implies a near linear hierarchical matrix type approximation of  $\Theta$  and  $A$ . This provides a direct link between our results and the more traditional wavelet based methods as a sparse counterpart of the hierarchical matrix method. Of course, these two approaches can not be expected to be fully equivalent. First of all, the fact that we chose the opposite elimination ordering for the Cholesky factorisation of sparse differential operators and their dense inverse, suggests that our method will not work well on sums of differential- and integral operators. For a SVD-based hierarchical compression, on the other hand, this should not pose any problem. Therefore, it seems likely that the hierarchical matrix method is more robust, than our sparsifying Cholesky factorisation. Furthermore, at least when using the SVD or analytic formulas to obtain the hierarchical matrix approximant, it should be able to avoid the artifact at the boundary when using the Matérn kernel, that we observe in Section 4.3.5. However, our method, in settings where it applies, has the advantage of constructing the sparse approximation from only linearly many entries of  $\Theta$  (the other entries do not need to be read, known or even stored), that are chosen independently of the Kernel. In contrast, if no analytic multipole expansion of the kernel is available and the hierarchical matrix approximants are computed via SVD, one needs to read every entry at least once and thus can not provide a near linear algorithm. To overcome this problem, other methods have been designed to compute the low-rank approximants in near-linear time. One approach is to use quadrature formulas (Fong and Darve, 2009) which require the evaluation of the covariance function at arbitrary points. Another possibility is to use rank-revealing  $LU$  decompositions (Miranian and Gu, 2003), rank-revealing  $QR$  decomposition (Gu and Eisenstat, 1996) or adaptive cross-approximation (Bebendorf and Rjasanow, 2003), which is very similar to rank-revealing  $LU$  decomposition. Quadrature based methods usually rely on having access to evaluations of the covariance at arbitrary points. Although methods based on rank-revealing factorisations only need to read a subset of the entries of the matrix, they are nonlinear and the required entries depend on the covariance matrix. For our method, in contrast, the relevant entries are known based only on the geometry of the measurement locations. This might be advantageous in settings, where the covariance matrix is estimated from a large number of realisations of the Gaussian process. In this case, to avoid having to store those realisations, one might resort to using the empirical covariance of the data. If this matrix is large as well, our method allows to discard all but near-linearly many entries which are known *a-priori*. A rank revealing  $LU$  decomposition instead, would need to see the covariance matrix before being able to decide, which entries need to be kept and which can be discarded.

## 5.2 Conclusion and outlook

To summarise, we have shown that when represented in a multi-resolution basis the Green's matrices of elliptic boundary value problems have exponentially localised Cholesky factorisations. Based on this result, we have shown that we can obtain a sparse approximation of this Cholesky factorisation, with the approximation error decaying exponentially in the size of the sparsity set. The computation of this decomposition can be equivalently expressed as a zero fill-in block-incomplete Cholesky factorisation of the truncated kernel matrix restricted to a sparsity set and can, for approximately equally spaced measurement locations and an approximation accuracy  $\epsilon$ , be computed in complexity  $\mathcal{O}\left(N \log^2(N) (\log(1/\epsilon) + \log^2(N))^{4d+1}\right)$  in time and  $\mathcal{O}(N \log(N) \log^d(N/\epsilon))$  in space. In particular,



only  $\mathcal{O}(N \log(N) \log^d(N/\epsilon))$  entries of the Kernel matrix expressed in the multiresolution basis need to be known for a reconstruction up to an error of size  $\epsilon$ . This appears to be a new type of rigidity result for the inverses of sparse matrices. Furthermore, our numerical evidence strongly suggests, that an elementwise incomplete Cholesky factorisation achieves an error of size  $\epsilon$  in complexity  $\mathcal{O}(N \log^2(N) \log^{2d}(N/\epsilon))$  in time and  $\mathcal{O}(N \log(N) \log^d(N/\epsilon))$  in space. In the case where  $s > d/2$ , that is when the solution space of the PDE contains continuous functions, we prove that a simple hierarchical ordering of the original matrix can be used as a *multi-resolution basis*. Therefore, this hierarchical ordering, by avoiding the need for aggregation in the multi-resolution transform, enables the exact change of basis in linear time and further strengthens our rigidity result (by implying that kernel matrices of this type are determined, up to an exponentially small errors, by near-linearly many of their entries, that in turn can be determined only based on the measurement locations).

Surprisingly, as a byproduct of our algorithm, we also obtain a sparse approximate principal component analysis in near-linear complexity, thereby opening the complexity bottleneck of this widely popular statistical procedure. Finally, as a corollary of our results, we obtain the existence of sparse approximants of the Cholesky factorisation of the inverse of the kernel matrix. More generally, we also observe a form of *duality* in the sense that for an ordering that leads to a sparse factorisation of the dense Green's matrix, the reverse ordering leads to a sparse factorisation of the associated stiffness matrix, which naturally leads to a fast direct solver for elliptic partial differential equations with rough coefficients.

The motivation for our sparse Cholesky decomposition has been the obvious, yet rarely used equivalence between the conditioning of gaussian vectors and the Cholesky factorisation of their covariance matrix. We suspect that this link between one of the most fundamental operations in computational mathematics — Gaussian elimination — and one of the most fundamental operations in statistics and probability — the conditioning of random variables — has not given all of its fruits yet.

In this work, we have left out a number of aspects that we deem interesting targets of future investigation:

1. We plan to provide a software package based on the results in this article. As part of this project, it will be interesting to compare different approaches for generating sparsifying orderings. Furthermore, it will be interesting to exploit the parallelism permitted by the locality of the factorisation.
2. In the article we have been dealing with point clouds in low-dimensional space. Since our algorithm only needs a notion of distance between points, it might be applicable to point clouds in high dimensional space, that have low intrinsic dimensionality, for example lying on low dimensional manifolds or having low doubling dimension. Preliminary results of this kind were provided in Section 4.3.4.
3. Somewhat related to the above point, we hope to be able to establish analogues of our method on graphs. The robustness of our algorithm and its independence from any notion of polynomials appears to suggest that it might be suited for this purpose than PDE based methods.
4. Some analytical questions might merit further investigation. These include the rigorous analysis of the case where  $2s$  is odd and the case where  $s$  is fractional. Furthermore, it is also of interest to examine to what extent subsampling is still feasible in the case  $s < d/2$ . Finally it might be possible to establish the stability result for incomplete Cholesky factorisation that allows for a rigorous error estimate for the element-wise factorisation.
5. In the wavelet literature (Gines et al., 1998), by using the so-called non-standard form, the complexity of the Cholesky decomposition for a fixed bandwidth can be reduced from  $\mathcal{O}(N \log^2(N))$  in time and  $\mathcal{O}(N \log(N))$  in space to  $\mathcal{O}(N)$  in time and space. We believe that in an analogous way a factor of  $\log(N)^2$ , resp.  $\log N$  can be dropped in our algorithm, as well, by using the non-standard form.
6. In the statistical literature, banded approximations of the Cholesky factors of the covariance matrix or its inverse have been used for the purpose of the estimation of covariance matrices (Bickel and Levina, 2008; Rothman et al., 2010; Fan et al., 2016). In this work we show that a large class of covariance matrices corresponding to smooth random fields can be very accurately approximated by

their truncated Cholesky factors. Therefore, it seems promising to investigate, whether truncated Cholesky factors (with the ordering and truncation pattern chosen as suggested in this work), can be useful as models for the estimation of covariance matrices.

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## References

- M. Abramowitz and I. A. Stegun. *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*, volume 55 of *National Bureau of Standards Applied Mathematics Series*. U.S. Government Printing Office, Washington, D.C., 1964.
- R. A. Adams and J. J. F. Fournier. *Sobolev Spaces*, volume 140 of *Pure and Applied Mathematics (Amsterdam)*. Elsevier/Academic Press, Amsterdam, second edition, 2003.
- S. Ambikasaran, D. Foreman-Mackey, L. Greengard, D. W. Hogg, and M. O’Neil. Fast direct methods for gaussian processes. *IEEE Trans. Pattern Anal. Mach. Intell.*, 38(2):252–265, 2016. doi:10.1109/TPAMI.2015.2448083.
- M. Armstrong. *Basic Linear Geostatistics*. Springer-Verlag, Berlin Heidelberg, 1998. doi:10.1007/978-3-642-58727-6.
- F. R. Bach and M. I. Jordan. Kernel independent component analysis. *J. Mach. Learn. Res.*, 3(1):1–48, 2003. doi:10.1162/153244303768966085.
- S. Banerjee, A. E. Gelfand, A. O. Finley, and H. Sang. Gaussian predictive process models for large spatial data sets. *J. R. Stat. Soc. Ser. B Stat. Methodol.*, 70(4):825–848, 2008. doi:10.1111/j.1467-9868.2008.00663.x.
- M. Bebendorf. Why finite element discretizations can be factored by triangular hierarchical matrices. *SIAM J. Numer. Anal.*, 45(4):1472–1494, 2007. doi:10.1137/060669747.
- M. Bebendorf. *Hierarchical Matrices*, volume 63 of *Lecture Notes in Computational Science and Engineering*. Springer-Verlag, Berlin, 2008. doi:10.1007/978-3-540-77147-0.
- M. Bebendorf. Low-rank approximation of elliptic boundary value problems with high-contrast coefficients. *SIAM J. Math. Anal.*, 48(2):932–949, 2016. doi:10.1137/140991030.
- M. Bebendorf and S. Rjasanow. Adaptive low-rank approximation of collocation matrices. *Computing*, 70(1):1–24, 2003. doi:10.1007/s00607-002-1469-6.
- M. Benzi. *Localization in Matrix Computations: Theory and Applications*, pages 211–317. Springer International Publishing, Cham, 2016. doi:10.1007/978-3-319-49887-4\_4.
- M. Benzi and M. Tuma. Orderings for factorized sparse approximate inverse preconditioners. *SIAM J. Sci. Comput.*, 21(5):1851–1868, 2000. doi:10.1137/S1064827598339372.
- C. Bernardi, Y. Maday, and F. Rapetti. *Discrétisations variationnelles de problèmes aux limites elliptiques*, volume 45 of *Mathématiques & Applications (Berlin) [Mathematics & Applications]*. Springer-Verlag, Berlin, 2004.
- G. Beylkin. On multiresolution methods in numerical analysis. In *Proceedings of the International Congress of Mathematicians, Vol. III (Berlin, 1998)*, number Extra Vol. III, pages 481–490, 1998.
- G. Beylkin and N. Coult. A multiresolution strategy for reduction of elliptic PDEs and eigenvalue problems. *Appl. Comput. Harmon. Anal.*, 5(2):129–155, 1998. doi:10.1006/acha.1997.0226.
- G. Beylkin, R. Coifman, and V. Rokhlin. Fast wavelet transforms and numerical algorithms. I. *Comm. Pure Appl. Math.*, 44(2):141–183, 1991. doi:10.1002/cpa.3160440202.
- P. J. Bickel and E. Levina. Regularized estimation of large covariance matrices. *Ann. Statist.*, 36(1): 199–227, 2008. doi:10.1214/009053607000000758.
- D. Bickson. Gaussian belief propagation: Theory and application, 2008. arXiv:0811.2518.

- S. Börm, L. Grasedyck, and W. Hackbusch. Introduction to hierarchical matrices with applications. *Eng. Anal. Bound. Elem.*, 27(5):405–422, 2003. doi:10.1016/S0955-7997(02)00152-2.
- D. Braess. *Finite Elements: Theory, Fast Solvers, and Applications in Elasticity Theory*. Cambridge University Press, Cambridge, third edition, 2007. doi:10.1017/CBO9780511618635. Translated from the German by Larry L. Schumaker.
- J. H. Bramble and S. R. Hilbert. Estimation of linear functionals on Sobolev spaces with application to Fourier transforms and spline interpolation. *SIAM J. Numer. Anal.*, 7:112–124, 1970. doi:10.1137/0707006.
- A. Brandt. Multi-level adaptive techniques (MLAT) for partial differential equations: ideas and software. pages 277–318. Publ. Math. Res. Center, No. 39, 1977.
- F.-X. Briol, C. J. Oates, M. Girolami, M. A. Osborne, and D. Sejdinovic. Probabilistic integration: A role for statisticians in numerical analysis?, 2015. arXiv:1512.00933.
- K. Chalupka, C. K. I. Williams, and I. Murray. A framework for evaluating approximation methods for Gaussian process regression. *J. Mach. Learn. Res.*, 14:333–350, 2013.
- J.-P. Chiles and P. Delfiner. *Geostatistics: Modeling Spatial Uncertainty*. Wiley Series in Probability and Statistics. John Wiley & Sons, Inc., Hoboken, NJ, second edition, 2012. doi:10.1002/9781118136188.
- O. A. Chkrebtii, D. A. Campbell, B. Calderhead, and M. A. Girolami. Bayesian solution uncertainty quantification for differential equations. *Bayesian Anal.*, 11(4):1239–1267, 2016. doi:10.1214/16-BA1017.
- J. Cockayne, C. Oates, T. J. Sullivan, and M. Girolami. Probabilistic meshless methods for partial differential equations and Bayesian inverse problems, 2016. arXiv:1605.07811.
- J. Cockayne, C. Oates, T. J. Sullivan, and M. Girolami. Bayesian probabilistic numerical methods, 2017. arXiv:1702.03673.
- P. R. Conrad, M. Girolami, S. Särkkä, A. M. Stuart, and K. C. Zygalakis. Statistical analysis of differential equations: introducing probability measures on numerical solutions. *Stat. Comput.*, 2016. doi:10.1007/s11222-016-9671-0.
- D. E. Crabtree and E. V. Haynsworth. An identity for the Schur complement of a matrix. *Proc. Amer. Math. Soc.*, 22:364–366, 1969. doi:10.2307/2037057.
- N. Cressie and G. Johannesson. Fixed rank kriging for very large spatial data sets. *J. R. Stat. Soc. Ser. B Stat. Methodol.*, 70(1):209–226, 2008. doi:10.1111/j.1467-9868.2007.00633.x.
- W. Dahmen, H. Harbrecht, and R. Schneider. Compression techniques for boundary integral equations— asymptotically optimal complexity estimates. *SIAM J. Numer. Anal.*, 43(6):2251–2271, 2006. doi:10.1137/S0036142903428852.
- Y. Daou and G. Stadler. Mitigating the influence of the boundary on PDE-based covariance operators, 2016. arXiv:1610.05280.
- I. Daubechies. *Ten Lectures on Wavelets*, volume 61 of *CBMS-NSF Regional Conference Series in Applied Mathematics*. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 1992. doi:10.1137/1.9781611970104.
- S. Dekel and D. Leviatan. The Bramble-Hilbert lemma for convex domains. *SIAM J. Math. Anal.*, 35(5):1203–1212, 2004. doi:10.1137/S0036141002417589.
- S. Demko, W. F. Moss, and P. W. Smith. Decay rates for inverses of band matrices. *Math. Comp.*, 43(168):491–499, 1984. doi:10.2307/2008290.
- R. A. DeVore and A. Kunoth, editors. *Multiscale, Nonlinear and Adaptive Approximation*. Springer-Verlag, Berlin Heidelberg, 2009. doi:10.1007/978-3-642-03413-8.
- P. Diaconis. Bayesian numerical analysis. In *Statistical decision theory and related topics, IV, Vol. 1 (West Lafayette, Ind., 1986)*, pages 163–175. Springer, New York, 1988.
- M. M. Dunlop, M. A. Iglesias, and A. M. Stuart. Hierarchical Bayesian level set inversion. *Stat. Comput.*, 2016. doi:10.1007/s11222-016-9704-8.
- J. Fan, Y. Liao, and H. Liu. An overview of the estimation of large covariance and precision matrices. *Econom. J.*, 19(1):C1–C32, 2016. doi:10.1111/ectj.12061.
- G. E. Fasshauer. Green’s functions: taking another look at kernel approximation, radial basis functions, and splines. In *Approximation theory XIII: San Antonio 2010*, volume 13 of *Springer Proc. Math.*, pages 37–63. Springer, New York, 2012. doi:10.1007/978-1-4614-0772-0\_4.
- R. P. Fedorenko. A relaxation method of solution of elliptic difference equations. *Ž. Vyčisl. Mat. i Mat. Fiz.*, 1:922–927, 1961.

- M. Feischl, T. Führer, N. Heuer, K. Michael, and D. Praetorius. Adaptive boundary element methods. *Arch. Comp. Meth. Eng.*, 22(3):309–389, 2015. doi:10.1007/s11831-014-9114-z.
- S. Fine and K. Scheinberg. Efficient svm training using low-rank kernel representations. *J. Mach. Learn. Res.*, 2:243–264, 2001. URL <http://www.jmlr.org/papers/volume2/fine01a/fine01a.pdf>.
- W. Fong and E. Darve. The black-box fast multipole method. *J. Comput. Phys.*, 228(23):8712–8725, 2009. doi:10.1016/j.jcp.2009.08.031.
- R. Furrer, M. G. Genton, and D. Nychka. Covariance tapering for interpolation of large spatial datasets. *J. Comput. Graph. Statist.*, 15(3):502–523, 2006. doi:10.1198/106186006X132178.
- J. Gallier. The Schur complement and symmetric positive semidefinite (and definite) matrices. *Penn Engineering*, 2010.
- T. Gantumur and R. P. Stevenson. Computation of singular integral operators in wavelet coordinates. *Computing*, 76(1-2):77–107, 2006. doi:10.1007/s00607-005-0135-1.
- A. George. Nested dissection of a regular finite element mesh. *SIAM J. Numer. Anal.*, 10:345–363, 1973. doi:10.1137/0710032.
- A. George and J. W. H. Liu. The evolution of the minimum degree ordering algorithm. *SIAM Rev.*, 31(1):1–19, 1989. doi:10.1137/1031001.
- J. R. Gilbert and R. E. Tarjan. The analysis of a nested dissection algorithm. *Numer. Math.*, 50(4):377–404, 1987. doi:10.1007/BF01396660.
- D. Gines, G. Beylkin, and J. Dunn. LU factorization of non-standard forms and direct multiresolution solvers. *Appl. Comput. Harmon. Anal.*, 5(2):156–201, 1998. doi:10.1006/acha.1997.0227.
- S. J. Gortler, P. Schröder, M. F. Cohen, and P. Hanrahan. Wavelet radiosity. In *Proceedings of the 20th Annual Conference on Computer Graphics and Interactive Techniques*, pages 221–230, 1993.
- L. Greengard and V. Rokhlin. A fast algorithm for particle simulations. *J. Comput. Phys.*, 73(2):325–348, 1987. doi:10.1016/0021-9991(87)90140-9.
- M. Gu and S. C. Eisenstat. Efficient algorithms for computing a strong rank-revealing QR factorization. *SIAM J. Sci. Comput.*, 17(4):848–869, 1996. doi:10.1137/0917055. URL <http://dx.doi.org/10.1137/0917055>.
- P. Guttorp and T. Gneiting. Studies in the history of probability and statistics. XLIX. On the Matérn correlation family. *Biometrika*, 93(4):989–995, 2006. doi:10.1093/biomet/93.4.989.
- W. Hackbusch. A fast iterative method for solving Poisson’s equation in a general region. pages 51–62. *Lecture Notes in Math.*, Vol. 631, 1978.
- W. Hackbusch. A sparse matrix arithmetic based on  $\mathcal{H}$ -matrices. I. Introduction to  $\mathcal{H}$ -matrices. *Computing*, 62(2):89–108, 1999. doi:10.1007/s006070050015.
- W. Hackbusch. *Multi-Grid Methods and Applications*, volume 4 of *Springer Series in Computational Mathematics*. Springer-Verlag, Berlin Heidelberg, 2013. doi:10.1007/978-3-662-02427-0.
- W. Hackbusch and S. Börm. Data-sparse approximation by adaptive  $\mathcal{H}^2$ -matrices. *Computing*, 69(1):1–35, 2002. doi:10.1007/s00607-002-1450-4.
- W. Hackbusch and B. N. Khoromskij. A sparse  $\mathcal{H}$ -matrix arithmetic. II. Application to multi-dimensional problems. *Computing*, 64(1):21–47, 2000.
- N. Halko, P.-G. Martinsson, and J. A. Tropp. Finding structure with randomness: probabilistic algorithms for constructing approximate matrix decompositions. *SIAM Rev.*, 53(2):217–288, 2011. doi:10.1137/090771806.
- H. Harbrecht. Preconditioning of wavelet BEM by the incomplete Cholesky factorization. *Comput. Vis. Sci.*, 15(6):319–329, 2012. doi:10.1007/s00791-014-0217-8.
- H. Harbrecht and R. Schneider. Wavelet Galerkin schemes for boundary integral equations—implementation and quadrature. *SIAM J. Sci. Comput.*, 27(4):1347–1370, 2006. doi:10.1137/S1064827503429387.
- P. Hennig. Probabilistic interpretation of linear solvers. *SIAM J. Optim.*, 25(1):234–260, 2015. doi:10.1137/140955501.
- P. Hennig, M. A. Osborne, and M. Girolami. Probabilistic numerics and uncertainty in computations. *Proc. A.*, 471(2179):20150142, 17, 2015. doi:10.1098/rspa.2015.0142.
- T. Y. Hou and P. Zhang. Sparse operator compression of higher order elliptic operators with rough coefficients. *to appear*, 2017.
- G. C. Hsiao. Boundary element methods—an overview. *Appl. Numer. Math.*, 56(10-11):1356–1369, 2006. doi:10.1016/j.apnum.2006.03.030.

- S. Jaffard. Propriétés des matrices “bien localisées” près de leur diagonale et quelques applications. volume 7, pages 461–476, 1990.
- A. G. Journel and C. J. Huijbregts. *Mining Geostatistics*. Academic Press, 1978.
- M. Katzfuss. A multi-resolution approximation for massive spatial datasets. *J. Amer. Stat. Assoc.*, 2016. doi:10.1080/01621459.2015.1123632.
- G. S. Kimeldorf and G. Wahba. A correspondence between Bayesian estimation on stochastic processes and smoothing by splines. *Ann. Math. Statist.*, 41:495–502, 1970.
- R. Kornhuber and H. Yserentant. An analysis of a class of variational multiscale methods based on subspace decomposition, 2016a. arXiv:1608.04081.
- R. Kornhuber and H. Yserentant. Numerical homogenization of elliptic multiscale problems by subspace decomposition. *Multiscale Model. Simul.*, 14(3):1017–1036, 2016b. doi:10.1137/15M1028510.
- I. Krishtal, T. Strohmer, and T. Wertz. Localization of matrix factorizations. *Found. Comput. Math.*, 15(4):931–951, 2015. doi:10.1007/s10208-014-9196-x.
- F. M. Larkin. Gaussian measure in Hilbert space and applications in numerical analysis. *Rocky Mountain J. Math.*, 2(3):379–421, 1972. doi:10.1216/RMJ-1972-2-3-379.
- F. Lindgren, H. Rue, and J. Lindström. An explicit link between Gaussian fields and Gaussian Markov random fields: the stochastic partial differential equation approach. *J. R. Stat. Soc. Ser. B Stat. Methodol.*, 73(4):423–498, 2011. doi:10.1111/j.1467-9868.2011.00777.x.
- R. J. Lipton, D. J. Rose, and R. E. Tarjan. Generalized nested dissection. *SIAM J. Numer. Anal.*, 16(2):346–358, 1979. doi:10.1137/0716027.
- S. Mallat. *A Wavelet Tour of Signal Processing*. Elsevier/Academic Press, Amsterdam, third edition, 2009. The sparse way, With contributions from Gabriel Peyré.
- B. Matérn. *Spatial Variation: Stochastic Models and Their Application to Some Problems in Forest Surveys and Other Sampling Investigations*. Meddelanden Fran Statens Skogsforskningsinstitut, Band 49, Nr.5, Stockholm, 1960.
- L. Miranian and M. Gu. Strong rank revealing *LU* factorizations. *Linear Algebra Appl.*, 367:1–16, 2003. doi:10.1016/S0024-3795(02)00572-4.
- D. Nychka, S. Bandyopadhyay, D. Hammerling, F. Lindgren, and S. Sain. A multiresolution Gaussian process model for the analysis of large spatial datasets. *J. Comput. Graph. Statist.*, 24(2):579–599, 2015. doi:10.1080/10618600.2014.914946.
- A. O’Hagan. Bayes–Hermite quadrature. *J. Statist. Plann. Inference*, 29(3):245–260, 1991. doi:10.1016/0378-3758(91)90002-V.
- A. O’Hagan. Some Bayesian numerical analysis. In J. M. Bernardo, J. O. Berger, A. P. Dawid, and A. F. M. Smith, editors, *Bayesian Statistics, 4: Proceedings of the Fourth Valencia International Meeting: Dedicated to the memory of Morris H. DeGroot, 1931–1989: April 15–20, 1991*, pages 345–363. Clarendon Press, 1992.
- H. Owhadi. Bayesian numerical homogenization. *Multiscale Model. Simul.*, 13(3):812–828, 2015. doi:10.1137/140974596.
- H. Owhadi. Multigrid with rough coefficients and multiresolution operator decomposition from hierarchical information games. *SIAM Rev.*, 59(1):99–149, 2017. doi:10.1137/15M1013894.
- H. Owhadi and C. Scovel. Conditioning Gaussian measure on Hilbert space, 2015. arXiv:1506.04208.
- H. Owhadi and C. Scovel. Universal scalable robust solvers from computational information games and fast eigenspace adapted multiresolution analysis, 2017. arXiv:1703.10761.
- P. Perdikaris, D. Venturi, and G. E. Karniadakis. Multifidelity information fusion algorithms for high-dimensional systems and massive data sets. *SIAM J. Sci. Comput.*, 38(4):B521–B538, 2016. doi:10.1137/15M1055164.
- H. Poincaré. *Calcul des probabilités*. Les Grands Classiques Gauthier-Villars. [Gauthier-Villars Great Classics]. Éditions Jacques Gabay, Sceaux, 1987. Reprint of the second (1912) edition.
- J. Quiñonero-Candela and C. E. Rasmussen. A unifying view of sparse approximate Gaussian process regression. *J. Mach. Learn. Res.*, 6(Dec):1939–1959, 2005. URL <http://www.jmlr.org/papers/volume6/quinonero-candela05a/quinonero-candela05a.pdf>.
- A. Rahimi and B. Recht. Random features for large-scale kernel machines. In J. C. Platt, D. Koller, Y. Singer, and S. T. Roweis, editors, *Advances in Neural Information Processing Systems 20*, pages 1177–1184. Curran Associates, Inc., 2008. URL <http://papers.nips.cc/paper/3182-random-features-for-large-scale-kernel-machines.pdf>.



- M. Raissi, P. Perdikaris, and G. E. Karniadakis. Inferring solutions of differential equations using noisy multi-fidelity data. *Journal of Computational Physics*, 335:736–746, 2017a. doi:10.1016/j.jcp.2017.01.060.
- M. Raissi, P. Perdikaris, and G. E. Karniadakis. Numerical Gaussian processes for time-dependent and non-linear partial differential equations, 2017b. arXiv:1703.10230.
- C. E. Rasmussen and C. K. I. Williams. *Gaussian Processes for Machine Learning*. Adaptive Computation and Machine Learning. MIT Press, Cambridge, MA, 2006.
- L. Roininen, M. S. Lehtinen, S. Lasanen, M. Orispää, and M. Markkanen. Correlation priors. *Inverse Probl. Imaging*, 5(1):167–184, 2011. doi:10.3934/ipi.2011.5.167.
- L. Roininen, P. Piiroinen, and M. Lehtinen. Constructing continuous stationary covariances as limits of the second-order stochastic difference equations. *Inverse Probl. Imaging*, 7(2):611–647, 2013. doi:10.3934/ipi.2013.7.611.
- L. Roininen, J. M. J. Huttunen, and S. Lasanen. Whittle-Matérn priors for Bayesian statistical inversion with applications in electrical impedance tomography. *Inverse Probl. Imaging*, 8(2):561–586, 2014. doi:10.3934/ipi.2014.8.561.
- A. J. Rothman, E. Levina, and J. Zhu. A new approach to Cholesky-based covariance regularization in high dimensions. *Biometrika*, 97(3):539–550, 2010. doi:10.1093/biomet/asq022.
- H. Sang and J. Z. Huang. A full scale approximation of covariance functions for large spatial data sets. *J. R. Stat. Soc. Ser. B. Stat. Methodol.*, 74(1):111–132, 2012. doi:10.1111/j.1467-9868.2011.01007.x.
- G. Santin and R. Schaback. Approximation of eigenfunctions in kernel-based spaces. *Adv. Comput. Math.*, 42(4):973–993, 2016. doi:10.1007/s10444-015-9449-5.
- A. Sard. *Linear Approximation*. American Mathematical Society, Providence, R.I., 1963.
- S. A. Sauter and C. Schwab. *Boundary Element Methods*, volume 39 of *Springer Series in Computational Mathematics*. Springer-Verlag, Berlin Heidelberg, 2011. doi:10.1007/978-3-540-68093-2.
- R. Schaback. A practical guide to radial basis functions. *Electronic Resource*, 2007.
- M. Schober, D. K. Duvenaud, and P. Hennig. Probabilistic ODE solvers with Runge–Kutta means. In Z. Ghahramani, M. Welling, C. Cortes, N. Lawrence, and K. Weinberger, editors, *Advances in Neural Information Processing Systems 27*, pages 739–747. Curran Associates, Inc., 2014. URL <http://papers.nips.cc/paper/5451-probabilistic-ode-solvers-with-runge-kutta-means>.
- B. Schölkopf and A. J. Smola. *Learning with Kernels: Support Vector Machines, Regularization, Optimization, and Beyond*. 2002.
- A. Schwaighofer and V. Tresp. Transductive and inductive methods for approximate Gaussian process regression. In S. Becker, S. Thrun, and K. Obermayer, editors, *Advances in Neural Information Processing Systems 15*, pages 977–984. MIT Press, 2003. URL <http://papers.nips.cc/paper/2230-transductive-and-inductive-methods-for-approximate-gaussian-process-regression.pdf>.
- J. E. H. Shaw. A quasirandom approach to integration in Bayesian statistics. *Ann. Statist.*, 16(2):895–914, 1988. doi:10.1214/aos/1176350842.
- J. R. Shewchuk et al. An introduction to the conjugate gradient method without the agonizing pain, 1994.
- J. Skilling. Bayesian solution of ordinary differential equations. In C. R. Smith, G. J. Erickson, and P. O. Neudorfer, editors, *Maximum Entropy and Bayesian Methods*, volume 50 of *Fundamental Theories of Physics*, pages 23–37. Springer, 1992. doi:10.1007/978-94-017-2219-3.
- A. J. Smola and B. Schölkopf. Sparse greedy matrix approximation for machine learning. In *Proceedings of the Seventeenth International Conference on Machine Learning*, pages 911–918, 2000.
- E. Snelson and Z. Ghahramani. Sparse Gaussian processes using pseudo-inputs. In Y. Weiss, P. B. Schölkopf, and J. C. Platt, editors, *Advances in Neural Information Processing Systems 18*, pages 1257–1264. MIT Press, 2006. URL <http://papers.nips.cc/paper/2857-sparse-gaussian-processes-using-pseudo-inputs.pdf>.
- M. L. Stein. *Interpolation of Spatial Data*. Springer Series in Statistics. Springer-Verlag, New York, 1999. doi:10.1007/978-1-4612-1494-6.
- M. L. Stein. The screening effect in kriging. *Ann. Statist.*, 30(1):298–323, 2002. doi:10.1214/aos/1015362194.
- M. L. Stein. Limitations on low rank approximations for covariance matrices of spatial data. *Spat. Stat.*, 8:1–19, 2014. doi:10.1016/j.spasta.2013.06.003.

- M. L. Stein, Z. Chi, and L. J. Welty. Approximating likelihoods for large spatial data sets. *J. R. Stat. Soc. Ser. B Stat. Methodol.*, 66(2):275–296, 2004. doi:10.1046/j.1369-7412.2003.05512.x.
- R. Stevenson. Adaptive wavelet methods for solving operator equations: an overview. In R. A. DeVore and A. Kunothe, editors, *Multiscale, Nonlinear and Adaptive Approximation*, pages 543–597. Springer, Berlin, 2009. doi:10.1007/978-3-642-03413-8\_13.
- A. M. Stuart. Inverse problems: a Bayesian perspective. *Acta Numer.*, 19:451–559, 2010. doi:10.1017/S0962492910000061.
- A. V. Sul’din. Wiener measure and its applications to approximation methods. I. *Izv. Vysš. Učebn. Zaved. Matematika*, 1959(6 (13)):145–158, 1959.
- M. K. Titsias. Variational learning of inducing variables in sparse Gaussian processes. In D. V. Dyk and M. Welling, editors, *Proceedings of the Twelfth International Conference on Artificial Intelligence and Statistics (AISTATS-09)*, volume 5, pages 567–574. Journal of Machine Learning Research — Proceedings Track, 2009. URL <http://jmlr.csail.mit.edu/proceedings/papers/v5/titsias09a/titsias09a.pdf>.
- H. Wendland. *Scattered Data Approximation*, volume 17 of *Cambridge Monographs on Applied and Computational Mathematics*. Cambridge University Press, Cambridge, 2005.
- P. Whittle. On stationary processes in the plane. *Biometrika*, 41:434–449, 1954. doi:10.1093/biomet/41.3-4.434.
- P. Whittle. Stochastic processes in several dimensions. *Bull. Inst. Internat. Statist.*, 40(2):974–994, 1963.
- C. K. I. Williams and M. Seeger. Using the Nyström method to speed up kernel machines. In T. K. Leen, T. G. Dietterich, and V. Tresp, editors, *Advances in Neural Information Processing Systems 13*, pages 682–688. MIT Press, 2001. URL <http://papers.nips.cc/paper/1866-using-the-nyström-method-to-speed-up-kernel-machines.pdf>.